



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:56 PM UTC

PDB ID : 1I1H / pdb_00001i1h
Title : CRYSTAL STRUCTURE ANALYSIS OF PRECORRIN-8X METHYLMUTASE COMPLEX WITH HYDROGENOBYRINIC ACID
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Deposited on : 2001-02-01
Resolution : 2.60 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

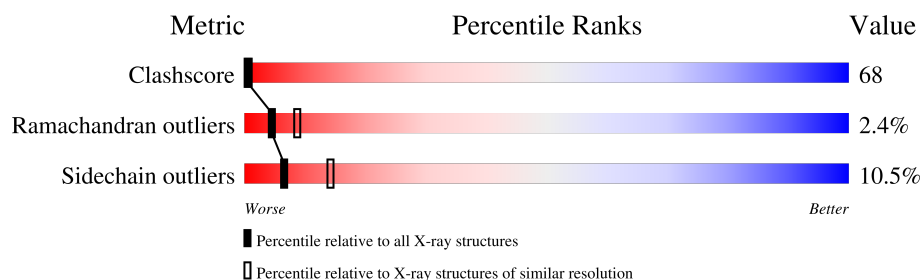
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	219	25% 59% 11% 5%

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	COJ	A	1121	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1720 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.

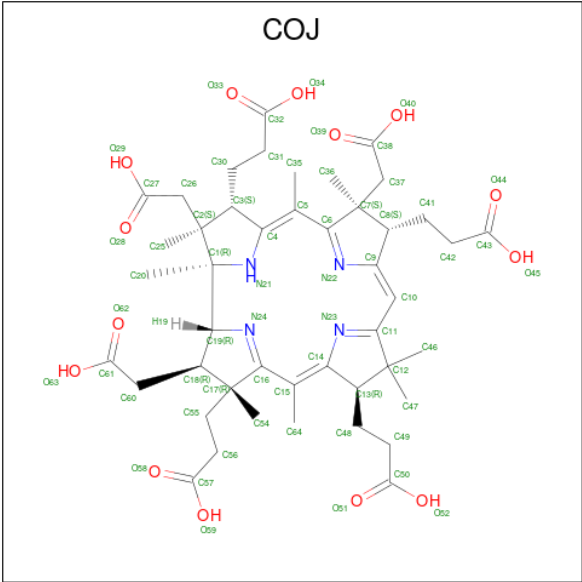
- Molecule 1 is a protein called PRECORRIN-8X METHYLMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1540	969	276	287	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP P21638
A	-7	ARG	-	expression tag	UNP P21638
A	-6	GLY	-	expression tag	UNP P21638
A	-5	SER	-	expression tag	UNP P21638
A	-4	HIS	-	expression tag	UNP P21638
A	-3	HIS	-	expression tag	UNP P21638
A	-2	HIS	-	expression tag	UNP P21638
A	-1	HIS	-	expression tag	UNP P21638
A	0	HIS	-	expression tag	UNP P21638
A	1	HIS	-	expression tag	UNP P21638

- Molecule 2 is HYDROGENOBYRINIC ACID (CCD ID: COJ) (formula: C₄₅H₆₀N₄O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			63	45	4	14		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		

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	90.10Å 36.60Å 60.30Å 90.00° 113.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1720	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: COJ

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	0.76	1/1568 (0.1%)	1.26	16/2127 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	MET	SD-CE	5.35	1.93	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	LEU	CA-C-N	7.54	129.27	119.84
1	A	90	LEU	C-N-CA	7.54	129.27	119.84
1	A	193	GLY	N-CA-C	-7.22	100.83	110.58
1	A	12	ALA	N-CA-C	-7.05	103.53	111.07
1	A	28	SER	N-CA-C	6.97	118.67	111.14
1	A	188	VAL	N-CA-C	-6.88	96.83	106.53
1	A	39	VAL	N-CA-C	6.64	117.39	110.62
1	A	80	MET	N-CA-C	-6.59	104.02	111.07
1	A	138	ALA	N-CA-C	6.43	122.65	108.64
1	A	72	ALA	CA-C-N	6.34	126.84	119.99
1	A	72	ALA	C-N-CA	6.34	126.84	119.99
1	A	186	ALA	N-CA-C	-6.00	98.01	110.80
1	A	65	ARG	N-CA-C	-5.79	105.06	111.71
1	A	153	ALA	CA-C-N	5.33	126.50	119.84
1	A	153	ALA	C-N-CA	5.33	126.50	119.84
1	A	165	GLY	N-CA-C	5.30	118.44	110.18

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	1540	0	1548	205	1
2	A	63	0	53	25	1
3	A	117	0	0	13	0
All	All	1720	0	1601	217	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 68.

All (217) 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:116:ARG:HH11	1:A:116:ARG:HG3	1.06	1.09
2:A:1121:COJ:C60	2:A:1121:COJ:H261	1.91	1.00
1:A:65:ARG:NH1	1:A:208:PRO:HG3	1.78	0.98
2:A:1121:COJ:H261	2:A:1121:COJ:H601	1.46	0.97
1:A:81:VAL:HG22	1:A:195:SER:HA	1.44	0.96
1:A:16:ARG:O	1:A:20:ILE:HG12	1.68	0.93
2:A:1121:COJ:H642	2:A:1121:COJ:H491	1.51	0.93
1:A:38:ALA:O	1:A:42:VAL:HG23	1.69	0.92
1:A:162:MET:HG2	1:A:188:VAL:HG23	1.52	0.91
1:A:86:THR:H	1:A:203:ASN:HD21	1.19	0.91
1:A:65:ARG:HH21	1:A:205:LEU:HA	1.37	0.89
1:A:129:ALA:HB3	3:A:1149:HOH:O	1.74	0.86
1:A:131:SER:HB3	3:A:1152:HOH:O	1.74	0.85
1:A:10:GLY:HA2	1:A:13:ILE:HD12	1.58	0.85
1:A:75:LEU:HD23	1:A:97:ILE:HB	1.58	0.84
1:A:73:PRO:HG3	1:A:127:ARG:HH21	1.41	0.84
2:A:1121:COJ:H351	2:A:1121:COJ:H363	1.58	0.83
1:A:101:ARG:HB2	3:A:1146:HOH:O	1.78	0.83
1:A:116:ARG:HG3	1:A:116:ARG:NH1	1.87	0.83
1:A:101:ARG:HB3	1:A:101:ARG:NH1	1.95	0.82
1:A:171:GLU:H	1:A:171:GLU:CD	1.88	0.82
1:A:65:ARG:HH12	1:A:208:PRO:HG3	1.44	0.81
1:A:130:GLY:C	1:A:157:ALA:HB2	2.06	0.81
1:A:195:SER:HB2	3:A:1238:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ALA:HA	2:A:1121:COJ:O45	1.82	0.79
1:A:91:PRO:HD3	1:A:206:ALA:HB1	1.65	0.79
1:A:196:ALA:HA	2:A:1121:COJ:C43	2.12	0.79
1:A:101:ARG:HB3	1:A:101:ARG:HH11	1.49	0.77
1:A:149:LEU:HA	1:A:153:ALA:HB3	1.65	0.77
1:A:31:SER:HB3	1:A:34:GLU:HG3	1.69	0.75
1:A:104:ARG:NH1	1:A:123:LEU:HG	2.02	0.74
1:A:65:ARG:NH2	1:A:205:LEU:HA	2.03	0.73
1:A:40:ARG:HH21	2:A:1121:COJ:H371	1.54	0.73
1:A:139:PRO:HB3	1:A:169:ALA:HA	1.69	0.73
2:A:1121:COJ:H353	2:A:1121:COJ:H302	1.69	0.72
1:A:69:LYS:HD3	3:A:1217:HOH:O	1.88	0.72
1:A:73:PRO:HG3	1:A:127:ARG:NH2	2.05	0.72
1:A:86:THR:OG1	2:A:1121:COJ:C35	2.38	0.72
1:A:158:ALA:O	1:A:159:ILE:HD13	1.89	0.71
1:A:142:LEU:HD21	1:A:176:LEU:HG	1.73	0.69
1:A:86:THR:OG1	2:A:1121:COJ:H353	1.92	0.69
1:A:69:LYS:HD2	1:A:91:PRO:HB3	1.72	0.69
1:A:42:VAL:HG13	1:A:47:SER:O	1.93	0.69
1:A:67:ALA:HB1	1:A:72:ALA:CB	2.23	0.69
1:A:45:CYS:SG	1:A:47:SER:HB3	2.33	0.69
1:A:36:ASP:OD2	1:A:208:PRO:HA	1.94	0.68
1:A:43:HIS:HE1	2:A:1121:COJ:H492	1.58	0.68
1:A:37:LEU:O	1:A:41:MET:HG3	1.95	0.67
1:A:128:LEU:O	1:A:156:PRO:HA	1.95	0.67
1:A:34:GLU:O	1:A:37:LEU:HB2	1.94	0.67
1:A:108:LEU:CB	1:A:119:ALA:HB1	2.26	0.66
1:A:17:SER:O	1:A:21:ILE:HG13	1.96	0.65
1:A:40:ARG:HD3	1:A:204:SER:HB2	1.78	0.64
1:A:60:PHE:CD2	1:A:186:ALA:HB2	2.32	0.64
1:A:159:ILE:HG12	1:A:183:VAL:HG21	1.79	0.63
1:A:121:LEU:HD11	1:A:141:ALA:O	2.00	0.61
1:A:6:TYR:HD2	1:A:6:TYR:H	1.47	0.61
1:A:77:ASP:CG	1:A:135:ILE:HA	2.26	0.61
1:A:108:LEU:HB3	1:A:119:ALA:HB1	1.82	0.61
2:A:1121:COJ:H261	2:A:1121:COJ:H602	1.80	0.61
1:A:9:ASP:OD1	1:A:12:ALA:HB2	2.00	0.60
1:A:60:PHE:CZ	1:A:160:LEU:HD13	2.37	0.60
1:A:49:GLU:HG3	3:A:1184:HOH:O	2.00	0.60
1:A:40:ARG:HH21	2:A:1121:COJ:C37	2.13	0.60
1:A:76:CYS:N	1:A:97:ILE:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLY:HA3	1:A:187:ILE:HG22	1.84	0.60
2:A:1121:COJ:H362	2:A:1121:COJ:H421	1.84	0.60
1:A:159:ILE:HG12	1:A:183:VAL:CG2	2.33	0.59
1:A:155:LYS:HB3	1:A:183:VAL:HG12	1.84	0.59
1:A:161:GLY:C	1:A:163:PRO:HD2	2.29	0.58
1:A:191:ARG:N	3:A:1125:HOH:O	2.36	0.58
1:A:161:GLY:O	1:A:187:ILE:HA	2.03	0.58
1:A:60:PHE:HB2	1:A:185:PHE:O	2.03	0.58
1:A:139:PRO:HD3	1:A:163:PRO:HB2	1.85	0.58
1:A:17:SER:OG	1:A:43:HIS:CE1	2.57	0.58
1:A:119:ALA:O	1:A:122:LYS:HG3	2.04	0.57
1:A:34:GLU:HG2	1:A:61:VAL:HG21	1.85	0.57
1:A:65:ARG:O	1:A:69:LYS:HB2	2.04	0.57
2:A:1121:COJ:H351	2:A:1121:COJ:C36	2.33	0.57
1:A:51:THR:HA	1:A:54:PHE:CD1	2.40	0.57
1:A:86:THR:CG2	1:A:89:ARG:HG3	2.35	0.57
1:A:31:SER:HB3	1:A:34:GLU:CG	2.35	0.57
1:A:81:VAL:HG22	1:A:195:SER:CA	2.28	0.57
1:A:32:GLU:HB3	3:A:1198:HOH:O	2.04	0.56
1:A:131:SER:N	1:A:157:ALA:H	2.02	0.56
1:A:199:ALA:HB3	2:A:1121:COJ:O45	2.05	0.56
1:A:122:LYS:O	1:A:125:SER:HB2	2.05	0.56
1:A:200:ALA:HA	2:A:1121:COJ:O39	2.06	0.56
1:A:86:THR:N	1:A:203:ASN:HD21	1.98	0.56
1:A:150:ARG:HB2	1:A:181:TYR:CZ	2.41	0.56
1:A:187:ILE:HD12	1:A:189:ARG:HG2	1.88	0.55
1:A:121:LEU:O	1:A:124:TRP:HB2	2.06	0.55
1:A:116:ARG:HH11	1:A:116:ARG:CG	1.94	0.55
1:A:7:ILE:HG13	3:A:1232:HOH:O	2.06	0.55
1:A:95:GLU:OE1	1:A:127:ARG:NH1	2.40	0.55
2:A:1121:COJ:H421	2:A:1121:COJ:C36	2.37	0.54
1:A:31:SER:O	1:A:33:GLU:N	2.41	0.54
1:A:162:MET:N	1:A:163:PRO:CD	2.71	0.54
1:A:31:SER:O	1:A:32:GLU:C	2.51	0.53
1:A:81:VAL:HA	3:A:1238:HOH:O	2.07	0.53
1:A:100:LEU:C	1:A:100:LEU:HD13	2.33	0.53
1:A:108:LEU:HB2	1:A:119:ALA:HB1	1.91	0.53
1:A:105:THR:HG21	1:A:120:ALA:HB2	1.90	0.53
1:A:187:ILE:CD1	1:A:189:ARG:HG2	2.39	0.53
1:A:73:PRO:CG	1:A:127:ARG:HH21	2.18	0.52
1:A:176:LEU:O	1:A:180:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:CG1	1:A:183:VAL:HG21	2.39	0.52
1:A:35:ALA:O	1:A:36:ASP:C	2.53	0.52
1:A:207:ARG:NH1	1:A:207:ARG:HG2	2.24	0.52
1:A:142:LEU:HD13	1:A:172:SER:C	2.34	0.51
1:A:131:SER:O	1:A:157:ALA:N	2.43	0.51
1:A:89:ARG:CZ	1:A:207:ARG:HG2	2.41	0.51
1:A:43:HIS:CE1	2:A:1121:COJ:H492	2.43	0.51
1:A:149:LEU:CA	1:A:153:ALA:HB3	2.37	0.51
1:A:86:THR:HG22	1:A:89:ARG:HG3	1.93	0.51
1:A:67:ALA:HB1	1:A:72:ALA:HB2	1.94	0.50
1:A:13:ILE:HD13	2:A:1121:COJ:O58	2.11	0.50
1:A:22:ARG:NH1	3:A:1204:HOH:O	2.37	0.50
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.77	0.50
1:A:57:SER:CB	1:A:185:PHE:H	2.24	0.50
1:A:203:ASN:OD1	2:A:1121:COJ:H363	2.11	0.50
1:A:150:ARG:HH21	1:A:151:ASP:CG	2.20	0.50
1:A:60:PHE:HZ	1:A:160:LEU:CD1	2.25	0.50
1:A:76:CYS:HA	1:A:134:ALA:O	2.13	0.49
1:A:10:GLY:CA	1:A:13:ILE:HD12	2.36	0.49
1:A:52:ARG:HG2	1:A:52:ARG:HH11	1.78	0.49
1:A:62:SER:O	1:A:66:ALA:HB2	2.13	0.49
1:A:89:ARG:NH1	1:A:203:ASN:O	2.43	0.49
1:A:31:SER:C	1:A:33:GLU:N	2.69	0.49
1:A:80:MET:HB2	1:A:195:SER:CB	2.43	0.49
1:A:56:PHE:CD1	1:A:56:PHE:N	2.80	0.49
1:A:94:ASN:HD22	1:A:94:ASN:H	1.59	0.49
1:A:183:VAL:HG23	1:A:184:PRO:O	2.13	0.49
1:A:40:ARG:O	1:A:43:HIS:HB3	2.13	0.48
1:A:77:ASP:OD1	1:A:135:ILE:HA	2.13	0.48
1:A:184:PRO:HG3	3:A:1122:HOH:O	2.13	0.48
1:A:139:PRO:CB	1:A:169:ALA:HA	2.42	0.48
1:A:49:GLU:O	1:A:52:ARG:HG3	2.12	0.48
1:A:121:LEU:HD12	1:A:144:PHE:HB3	1.95	0.48
1:A:203:ASN:HB2	2:A:1121:COJ:O39	2.14	0.48
1:A:31:SER:O	1:A:34:GLU:N	2.47	0.48
1:A:55:VAL:O	1:A:186:ALA:HA	2.13	0.48
1:A:49:GLU:O	1:A:50:ALA:C	2.56	0.47
1:A:171:GLU:CD	1:A:171:GLU:N	2.62	0.47
1:A:45:CYS:SG	1:A:197:MET:HE2	2.54	0.47
1:A:60:PHE:CE2	1:A:186:ALA:HB2	2.49	0.47
1:A:37:LEU:HD12	1:A:41:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:CG1	1:A:48:VAL:HA	2.44	0.47
1:A:90:LEU:HD22	1:A:94:ASN:HB2	1.97	0.47
1:A:161:GLY:N	1:A:186:ALA:O	2.45	0.47
1:A:18:PHE:CD2	1:A:210:LEU:HD21	2.50	0.47
1:A:99:THR:OG1	1:A:120:ALA:HB1	2.15	0.47
1:A:124:TRP:O	1:A:127:ARG:N	2.47	0.47
1:A:144:PHE:CE2	1:A:148:MET:HE3	2.50	0.47
1:A:164:VAL:HB	1:A:193:GLY:C	2.41	0.46
1:A:77:ASP:OD2	1:A:138:ALA:N	2.49	0.46
1:A:57:SER:OG	1:A:184:PRO:HB3	2.15	0.46
1:A:145:LEU:HD13	1:A:149:LEU:HD11	1.98	0.46
1:A:86:THR:HG22	1:A:86:THR:O	2.15	0.46
1:A:54:PHE:C	1:A:55:VAL:HG23	2.40	0.45
1:A:60:PHE:CZ	1:A:160:LEU:CD1	2.99	0.45
1:A:42:VAL:HG13	1:A:48:VAL:HA	1.99	0.45
1:A:90:LEU:HD13	1:A:94:ASN:O	2.17	0.45
1:A:74:ILE:HD13	1:A:202:LEU:HD22	1.98	0.45
1:A:53:GLN:O	1:A:55:VAL:HG23	2.16	0.45
1:A:80:MET:HB2	1:A:195:SER:HB3	1.98	0.45
1:A:76:CYS:HB2	1:A:98:CYS:HB2	1.98	0.44
2:A:1121:COJ:H461	2:A:1121:COJ:H481	1.56	0.44
1:A:135:ILE:HG22	1:A:163:PRO:HB3	1.99	0.44
1:A:149:LEU:HD21	1:A:156:PRO:HD3	2.00	0.44
1:A:134:ALA:HA	1:A:160:LEU:HB2	2.00	0.44
1:A:208:PRO:O	1:A:209:GLY:C	2.59	0.44
1:A:62:SER:OG	1:A:63:SER:N	2.51	0.44
1:A:138:ALA:HA	1:A:139:PRO:HD2	1.95	0.44
1:A:142:LEU:HB3	1:A:172:SER:HB2	2.00	0.43
1:A:73:PRO:CG	1:A:127:ARG:NH2	2.77	0.43
1:A:90:LEU:HA	1:A:91:PRO:HD3	1.76	0.43
1:A:136:GLY:HA3	1:A:198:THR:OG1	2.19	0.43
1:A:20:ILE:O	1:A:24:GLU:HG3	2.18	0.43
1:A:91:PRO:HD2	1:A:94:ASN:ND2	2.34	0.43
1:A:176:LEU:HD13	1:A:185:PHE:HB2	2.00	0.43
1:A:11:ASN:H	1:A:11:ASN:HD22	1.66	0.42
1:A:112:ILE:HD12	1:A:112:ILE:N	2.34	0.42
1:A:118:ALA:O	1:A:119:ALA:C	2.61	0.42
1:A:63:SER:O	1:A:66:ALA:HB3	2.20	0.42
1:A:57:SER:HB3	1:A:185:PHE:H	1.83	0.42
1:A:37:LEU:HB3	1:A:41:MET:HE3	2.01	0.42
2:A:1121:COJ:H601	2:A:1121:COJ:C26	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:O	1:A:116:ARG:C	2.62	0.42
1:A:145:LEU:HD13	1:A:149:LEU:CD1	2.50	0.42
1:A:92:ALA:O	1:A:93:GLY:C	2.62	0.41
1:A:147:GLU:O	1:A:148:MET:C	2.61	0.41
1:A:67:ALA:C	1:A:69:LYS:N	2.78	0.41
1:A:89:ARG:NH1	1:A:89:ARG:HB3	2.35	0.41
1:A:139:PRO:HG3	1:A:169:ALA:CA	2.50	0.41
1:A:16:ARG:O	1:A:16:ARG:HG2	2.19	0.41
1:A:86:THR:O	1:A:87:ARG:C	2.63	0.41
1:A:94:ASN:H	1:A:94:ASN:ND2	2.18	0.41
1:A:105:THR:HG23	1:A:120:ALA:CA	2.51	0.41
1:A:135:ILE:HG22	1:A:135:ILE:O	2.21	0.41
1:A:189:ARG:NH2	3:A:1233:HOH:O	2.52	0.41
1:A:121:LEU:HD23	1:A:124:TRP:CE2	2.56	0.41
1:A:173:LYS:NZ	1:A:190:GLY:O	2.35	0.41
1:A:128:LEU:O	1:A:129:ALA:C	2.64	0.41
1:A:105:THR:O	1:A:106:PRO:C	2.63	0.41
1:A:155:LYS:HB3	1:A:183:VAL:CG1	2.49	0.41
2:A:1121:COJ:H262	2:A:1121:COJ:H19	1.62	0.41
1:A:130:GLY:CA	1:A:157:ALA:HB2	2.50	0.40
1:A:138:ALA:O	1:A:141:ALA:HB3	2.21	0.40
1:A:105:THR:HG23	1:A:120:ALA:HA	2.03	0.40
1:A:161:GLY:C	1:A:163:PRO:CD	2.94	0.40
1:A:209:GLY:O	1:A:210:LEU:HD23	2.21	0.40
1:A:18:PHE:HZ	1:A:40:ARG:NH1	2.20	0.40
1:A:27:LEU:HD11	1:A:39:VAL:HG22	2.04	0.40
1:A:124:TRP:CZ3	1:A:133:VAL:HG22	2.57	0.40
1:A:161:GLY:CA	1:A:187:ILE:HG22	2.49	0.40
1:A:68:LEU:CD2	1:A:206:ALA:HB2	2.51	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:A:116:ARG:NH2	2:A:1121:COJ:O29[2_655]	2.11	0.09

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	124/219 (57%)	105 (85%)	16 (13%)	3 (2%)	4 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	SER
1	A	32	GLU
1	A	58	PRO

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	152/161 (94%)	136 (90%)	16 (10%)	6 14

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	58	PRO
1	A	80	MET
1	A	104	ARG
1	A	114	ASN
1	A	116	ARG
1	A	117	SER
1	A	123	LEU

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Mol	Chain	Res	Type
1	A	125	SER
1	A	142	LEU
1	A	160	LEU
1	A	171	GLU
1	A	176	LEU
1	A	183	VAL
1	A	195	SER
1	A	207	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	43	HIS
1	A	94	ASN
1	A	203	ASN

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](#)

1 ligand is 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
2	COJ	A	1121	-	61,67,67	2.38	23 (37%)	76,106,106	2.38	18 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COJ	A	1121	-	-	11/49/145/145	0/4/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1121	COJ	C20-C1	7.22	1.59	1.52
2	A	1121	COJ	C13-C14	6.36	1.59	1.51
2	A	1121	COJ	C17-C18	5.65	1.65	1.54
2	A	1121	COJ	C55-C17	3.81	1.63	1.54
2	A	1121	COJ	C14-N23	-3.61	1.30	1.37
2	A	1121	COJ	C26-C2	3.59	1.64	1.55
2	A	1121	COJ	C4-N21	-3.50	1.27	1.32
2	A	1121	COJ	C31-C32	3.43	1.58	1.50
2	A	1121	COJ	C15-C14	3.36	1.45	1.38
2	A	1121	COJ	C48-C13	3.12	1.61	1.54
2	A	1121	COJ	C3-C4	3.01	1.58	1.52
2	A	1121	COJ	C6-N22	3.01	1.43	1.33
2	A	1121	COJ	C25-C2	2.91	1.59	1.54
2	A	1121	COJ	C30-C3	2.89	1.61	1.54
2	A	1121	COJ	C19-N24	2.69	1.51	1.47
2	A	1121	COJ	C64-C15	2.66	1.56	1.50
2	A	1121	COJ	C26-C27	2.36	1.57	1.50
2	A	1121	COJ	O33-C32	2.33	1.29	1.22
2	A	1121	COJ	C11-N23	-2.32	1.28	1.33
2	A	1121	COJ	C54-C17	2.20	1.58	1.54
2	A	1121	COJ	C41-C8	2.20	1.59	1.54
2	A	1121	COJ	O44-C43	2.18	1.29	1.22
2	A	1121	COJ	O59-C57	-2.04	1.24	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1121	COJ	C14-N23-C11	7.72	116.41	108.39
2	A	1121	COJ	C20-C1-N21	-7.08	101.81	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1121	COJ	C17-C16-C15	6.65	136.47	126.03
2	A	1121	COJ	C7-C6-C5	5.14	134.11	126.03
2	A	1121	COJ	C56-C55-C17	4.90	125.04	115.58
2	A	1121	COJ	C6-N22-C9	4.63	113.06	108.27
2	A	1121	COJ	C55-C17-C16	4.44	125.28	116.59
2	A	1121	COJ	C60-C18-C17	4.29	127.56	115.82
2	A	1121	COJ	C20-C1-C2	-4.11	102.02	114.64
2	A	1121	COJ	C1-C19-N24	3.65	116.92	112.12
2	A	1121	COJ	C48-C13-C14	3.63	124.43	111.85
2	A	1121	COJ	C54-C17-C55	-3.58	103.32	109.27
2	A	1121	COJ	C49-C48-C13	3.34	124.13	114.65
2	A	1121	COJ	C13-C14-N23	-2.97	107.89	111.95
2	A	1121	COJ	C48-C13-C12	-2.67	108.88	116.52
2	A	1121	COJ	C64-C15-C14	-2.22	111.05	120.90
2	A	1121	COJ	C25-C2-C26	-2.13	105.51	109.74
2	A	1121	COJ	C13-C14-C15	2.09	131.33	125.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1121	COJ	C14-C13-C48-C49
2	A	1121	COJ	C18-C17-C55-C56
2	A	1121	COJ	C16-C17-C55-C56
2	A	1121	COJ	C54-C17-C55-C56
2	A	1121	COJ	C12-C13-C48-C49
2	A	1121	COJ	C17-C55-C56-C57
2	A	1121	COJ	C17-C18-C60-C61
2	A	1121	COJ	C48-C49-C50-O51
2	A	1121	COJ	C48-C49-C50-O52
2	A	1121	COJ	C30-C31-C32-O34
2	A	1121	COJ	C30-C31-C32-O33

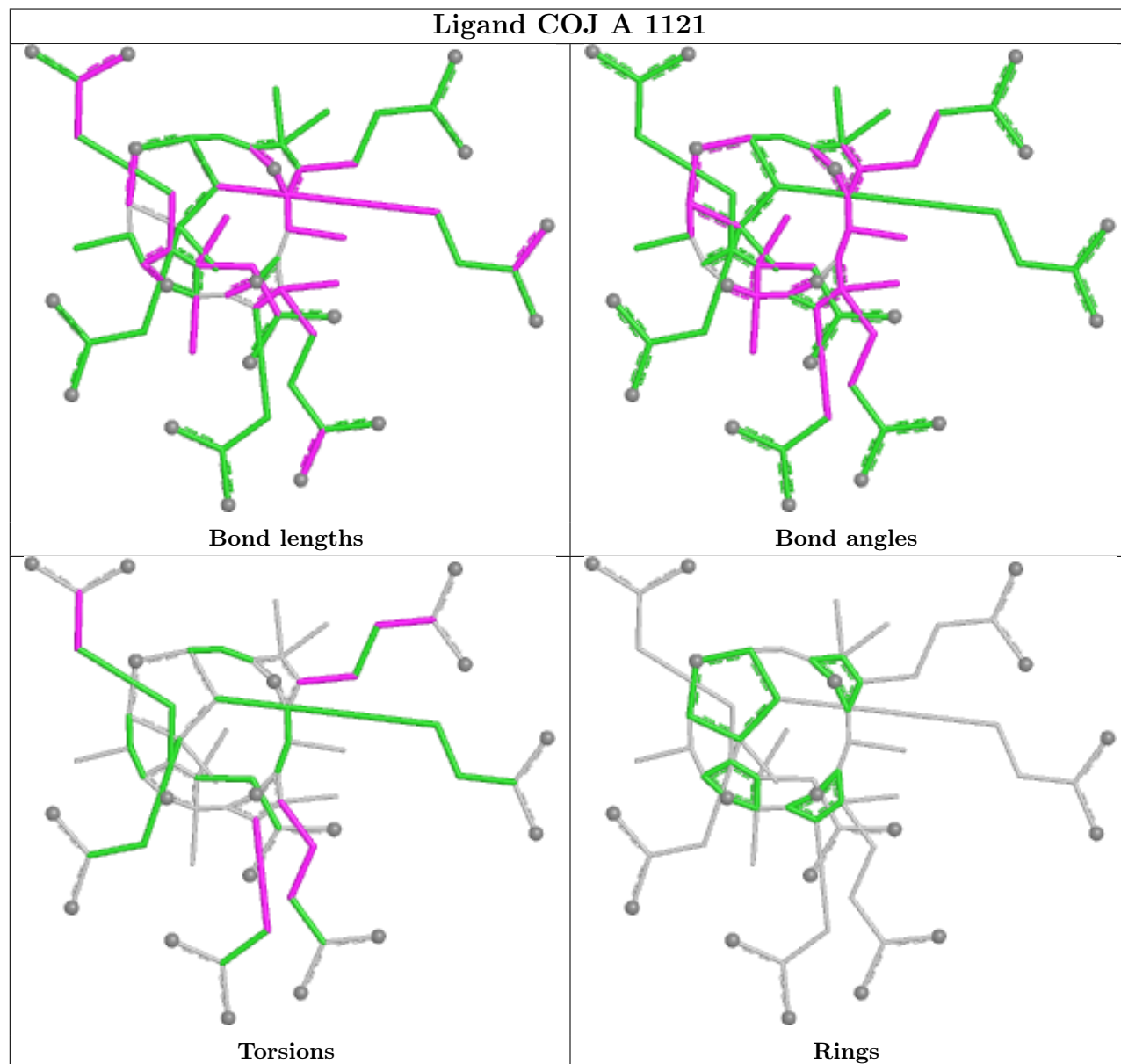
There are no ring outliers.

1 monomer is involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1121	COJ	25	1

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 ⓘ

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.