



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:56 AM UTC

PDB ID : 1W6S / pdb_00001w6s
Title : The high resolution structure of methanol dehydrogenase from methylobacterium extorquens
Authors : Williams, P.A.; Coates, L.; Mohammed, F.; Gill, R.; Erskine, P.T.; Wood, S.P.; Anthony, C.; Cooper, J.B.
Deposited on : 2004-08-23
Resolution : 1.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

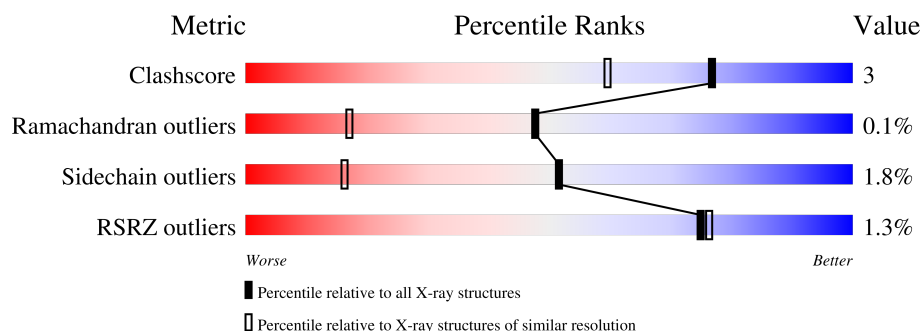
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	599	0% 89% 9% ..
1	C	599	2% 90% 9% .
2	B	74	3% 85% 12% ..
2	D	74	3% 84% 14% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1597	-	X	-	-
4	GOL	A	1598	-	X	-	-
4	GOL	C	3598	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11845 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 METHANOL DEHYDROGENASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	1
			4607	2938	774	875	20			
1	C	597	Total	C	N	O	S	0	0	1
			4601	2932	772	877	20			

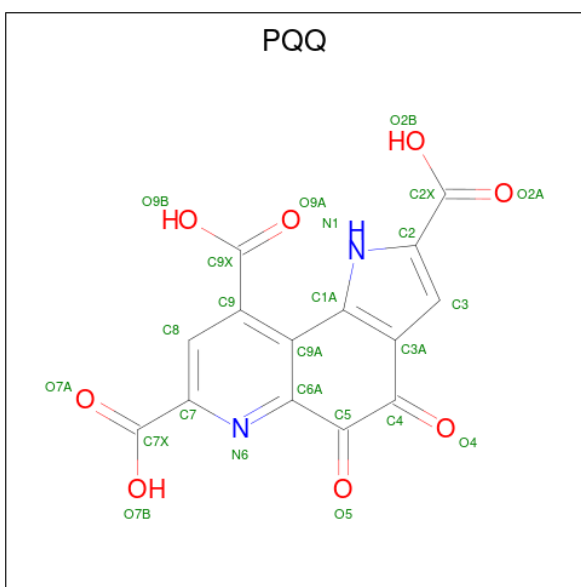
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	LYS	ARG	conflict	UNP P16027
C	2426	LYS	ARG	conflict	UNP P16027

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	1
			574	361	102	108	3			
2	D	73	Total	C	N	O	S	0	0	1
			558	349	98	108	3			

- Molecule 3 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: C₁₄H₆N₂O₈).



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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

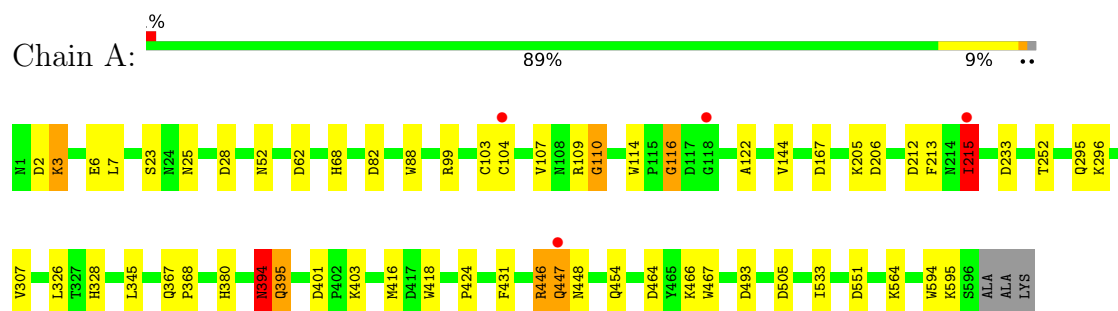
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	605	Total	O	0	0
			605	605		
6	B	133	Total	O	0	0
			133	133		
6	C	610	Total	O	0	0
			610	610		
6	D	89	Total	O	0	0
			89	89		

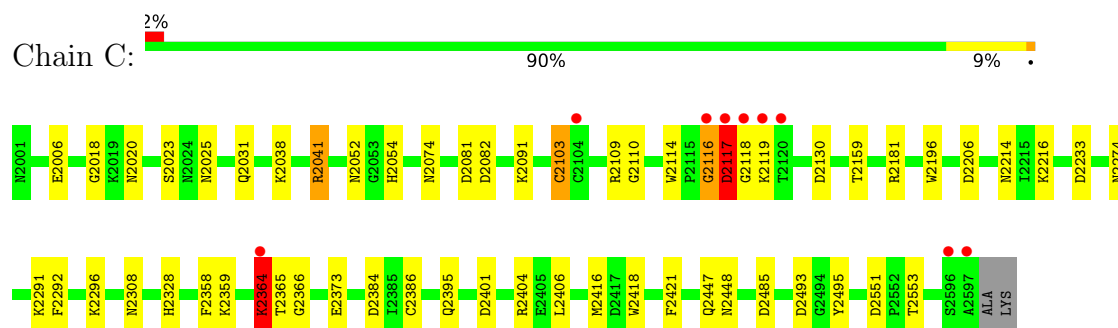
3 Residue-property plots

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

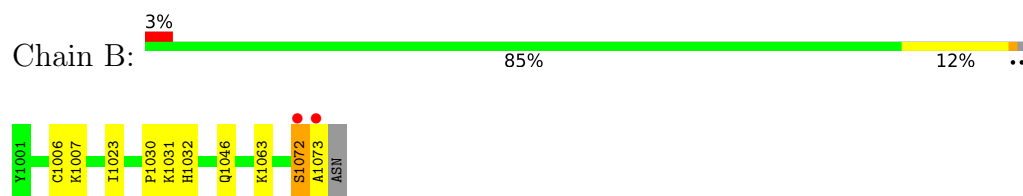
• Molecule 1: METHANOL DEHYDROGENASE SUBUNIT 1



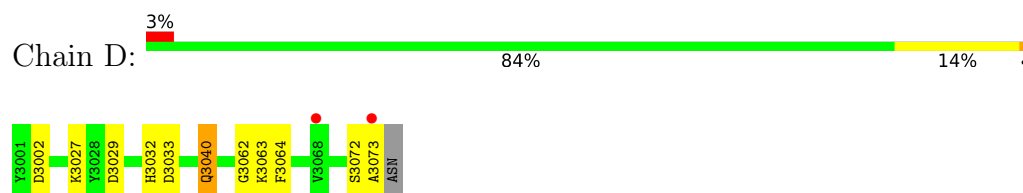
• Molecule 1: METHANOL DEHYDROGENASE SUBUNIT 1



• Molecule 2: METHANOL DEHYDROGENASE SUBUNIT 2



• Molecule 2: METHANOL DEHYDROGENASE SUBUNIT 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.90Å 73.62Å 88.08Å 86.09° 104.11° 109.68°	Depositor
Resolution (Å)	10.00 – 1.20 10.00 – 1.23	Depositor EDS
% Data completeness (in resolution range)	85.0 (10.00-1.20) 84.9 (10.00-1.23)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.23Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.153 , 0.177 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 90.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11845	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, PQQ

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	1.34	4/4737 (0.1%)	1.66	51/6443 (0.8%)
1	C	1.34	5/4731 (0.1%)	1.65	60/6439 (0.9%)
2	B	1.04	1/587 (0.2%)	1.50	2/784 (0.3%)
2	D	0.79	0/570	1.59	8/766 (1.0%)
All	All	1.30	10/10625 (0.1%)	1.64	121/14432 (0.8%)

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
1	A	0	1
1	C	0	3
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2117	ASP	CG-OD2	25.17	1.73	1.25
1	C	2117	ASP	CB-CG	14.48	1.88	1.52
1	A	215	ILE	CG1-CD1	9.67	1.89	1.51
1	C	2117	ASP	CG-OD1	-7.43	1.11	1.25
1	A	215	ILE	CB-CG1	-5.80	1.41	1.53
1	C	2386	CYS	CA-C	5.74	1.57	1.52
1	A	595	LYS	C-N	-5.42	1.25	1.33
1	C	2364	LYS	CE-NZ	5.27	1.65	1.49
1	A	144	VAL	C-O	5.25	1.29	1.23
2	B	1072	SER	C-N	-5.19	1.26	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	GLN	OE1-CD-NE2	-22.36	100.24	122.60
1	A	215	ILE	CB-CG1-CD1	-17.42	77.22	113.80
1	C	2117	ASP	CB-CG-OD2	-15.90	81.84	118.40
1	A	447	GLN	CG-CD-NE2	13.21	136.22	116.40
1	C	2448	ASN	CA-CB-CG	11.56	124.17	112.60
1	A	551	ASP	CA-CB-CG	10.83	123.43	112.60
1	C	2117	ASP	CA-CB-CG	-10.25	102.35	112.60
1	C	2384	ASP	N-CA-CB	-10.16	96.79	112.13
1	C	2117	ASP	N-CA-CB	9.14	125.94	110.49
1	C	2493	ASP	CA-CB-CG	8.74	121.34	112.60
1	A	394	ASN	OD1-CG-ND2	-8.45	114.15	122.60
1	C	2110	GLY	N-CA-C	8.13	120.98	111.63
1	C	2448	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	C	2418	TRP	CA-CB-CG	7.84	128.49	113.60
1	A	493	ASP	CA-CB-CG	7.82	120.42	112.60
1	A	418	TRP	CA-CB-CG	7.81	128.45	113.60
1	A	447	GLN	CB-CG-CD	-7.56	99.75	112.60
1	A	116	GLY	CA-C-O	-7.52	117.04	122.23
1	C	2116	GLY	CA-C-O	7.51	128.38	122.29
2	B	1006	CYS	O-C-N	-7.36	114.73	123.27
1	A	394	ASN	CA-CB-CG	7.28	119.88	112.60
1	A	215	ILE	CG1-CB-CG2	-7.27	88.88	110.70
1	A	99	ARG	CD-NE-CZ	7.24	134.54	124.40
1	C	2082	ASP	CA-CB-CG	7.24	119.84	112.60
1	C	2401	ASP	CA-CB-CG	7.14	119.74	112.60
1	A	446	ARG	CD-NE-CZ	7.12	134.37	124.40
1	C	2274	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	C	2117	ASP	CB-CA-C	-6.91	96.67	110.42
1	C	2116	GLY	CA-C-N	-6.87	108.42	121.54
1	C	2116	GLY	C-N-CA	-6.87	108.42	121.54
1	C	2117	ASP	CB-CG-OD1	6.86	134.17	118.40
1	C	2416	MET	N-CA-C	6.85	119.48	109.07
1	C	2025	ASN	CA-CB-CG	6.83	119.43	112.60
1	C	2366	GLY	O-C-N	-6.82	113.73	122.39
1	C	2485	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	431	PHE	CA-CB-CG	6.76	120.56	113.80
1	C	2384	ASP	CB-CA-C	6.69	121.24	111.73
1	A	403	LYS	CA-C-O	-6.64	112.86	120.24
1	C	2109	ARG	CG-CD-NE	-6.55	97.58	112.00
1	C	2031	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	A	109	ARG	CG-CD-NE	-6.47	97.77	112.00
1	A	467	TRP	CA-CB-CG	6.45	125.85	113.60
1	A	88	TRP	CA-CB-CG	6.44	125.84	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2364	LYS	CG-CD-CE	6.43	126.10	111.30
1	C	2358	PHE	CA-CB-CG	6.39	120.19	113.80
1	C	2551	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	104	CYS	N-CA-CB	-6.31	104.22	111.79
1	A	505	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	380	HIS	CA-CB-CG	6.22	120.02	113.80
1	A	416	MET	N-CA-C	6.21	118.52	109.07
1	C	2447	GLN	CB-CG-CD	6.21	123.16	112.60
1	A	52	ASN	CA-CB-CG	6.20	118.80	112.60
1	C	2364	LYS	CB-CA-C	6.16	120.03	109.24
2	D	3033	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	446	ARG	O-C-N	-6.11	114.03	122.46
1	C	2216	LYS	CA-C-N	6.07	129.69	122.89
1	C	2216	LYS	C-N-CA	6.07	129.69	122.89
1	A	326	LEU	CA-C-O	-6.00	114.33	121.11
1	C	2074	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	110	GLY	N-CA-C	5.85	119.28	110.97
1	A	213	PHE	CA-C-N	5.85	130.89	122.40
1	A	213	PHE	C-N-CA	5.85	130.89	122.40
1	A	401	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	206	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	594	TRP	O-C-N	-5.81	115.81	122.89
2	D	3002	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	2406	LEU	CA-C-N	5.74	130.28	122.19
1	C	2406	LEU	C-N-CA	5.74	130.28	122.19
1	C	2214	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	C	2081	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	2308	ASN	CA-C-N	5.72	128.39	120.49
1	C	2308	ASN	C-N-CA	5.72	128.39	120.49
1	A	2	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	233	ASP	CA-CB-CG	5.69	118.29	112.60
2	D	3063	LYS	O-C-N	-5.65	116.71	123.27
1	C	2292	PHE	CA-CB-CG	5.59	119.39	113.80
1	A	454	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	C	2109	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	C	2041	ARG	CA-CB-CG	5.58	125.25	114.10
1	C	2421	PHE	CA-CB-CG	5.56	119.36	113.80
1	C	2206	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	2159	THR	O-C-N	-5.52	116.25	122.10
1	A	28	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	2373	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	252	THR	CA-C-N	5.38	131.49	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	THR	C-N-CA	5.38	131.49	123.05
1	C	2109	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	394	ASN	O-C-N	-5.35	115.48	122.59
1	A	307	VAL	N-CA-C	5.34	118.95	112.80
1	C	2130	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	2233	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	82	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	368	PRO	CA-C-O	-5.29	114.96	121.31
2	D	3064	PHE	N-CA-C	5.25	117.84	109.96
1	A	104	CYS	CA-C-N	5.25	131.56	121.54
1	A	104	CYS	C-N-CA	5.25	131.56	121.54
1	C	2364	LYS	CD-CE-NZ	5.24	128.66	111.90
1	C	2025	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	C	2196	TRP	CA-CB-CG	5.22	123.52	113.60
1	A	167	ASP	CA-CB-CG	5.18	117.78	112.60
2	D	3062	GLY	CA-C-N	5.17	130.29	123.00
2	D	3062	GLY	C-N-CA	5.17	130.29	123.00
1	C	2091	LYS	CA-C-N	5.17	125.08	119.76
1	C	2091	LYS	C-N-CA	5.17	125.08	119.76
2	B	1046	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	C	2103	CYS	N-CA-CB	5.15	117.78	110.16
1	A	122	ALA	CA-C-O	-5.14	115.54	121.19
1	A	367	GLN	CA-C-O	-5.13	115.88	120.19
1	C	2404	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	D	3040	GLN	O-C-N	-5.12	115.97	122.27
1	C	2018	GLY	CA-C-N	5.12	131.32	121.54
1	C	2018	GLY	C-N-CA	5.12	131.32	121.54
1	A	295	GLN	CA-C-N	5.12	127.56	120.29
1	A	295	GLN	C-N-CA	5.12	127.56	120.29
1	A	213	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	2054	HIS	CG-CD2-NE2	5.09	112.29	107.20
2	D	3029	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	25	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	2020	ASN	CA-C-O	-5.03	116.07	121.45
1	A	107	VAL	N-CA-C	5.01	115.52	110.05
1	C	2052	ASN	OD1-CG-ND2	-5.00	117.60	122.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	C	2103	CYS	Peptide
1	C	2117	ASP	Sidechain
1	C	2495	TYR	Peptide

5.2 Too-close contacts [i](#)

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	4607	0	4406	24	0
1	C	4601	0	4375	20	0
2	B	574	0	561	5	0
2	D	558	0	517	6	0
3	A	24	0	3	0	0
3	C	24	0	5	0	0
4	A	12	0	11	3	0
4	C	6	0	5	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	605	0	0	9	0
6	B	133	0	0	2	0
6	C	610	0	0	5	0
6	D	89	0	0	0	0
All	All	11845	0	9883	58	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 3.

All (58) 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:215:ILE:HG21	1:A:215:ILE:CD1	1.32	1.59
1:A:215:ILE:HD13	1:A:215:ILE:CG2	1.41	1.49
1:A:215:ILE:CD1	1:A:215:ILE:CG1	1.89	1.47
1:C:2117:ASP:CB	1:C:2117:ASP:CG	1.88	1.46
1:A:215:ILE:CD1	1:A:215:ILE:CG2	1.94	1.40
4:C:3598:GOL:O3	4:C:3598:GOL:C3	1.77	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1597:GOL:C3	4:A:1597:GOL:O3	1.75	1.32
1:C:2117:ASP:CG	1:C:2117:ASP:OD2	1.73	1.31
4:A:1598:GOL:C3	4:A:1598:GOL:O3	1.79	1.31
1:A:215:ILE:CD1	1:A:215:ILE:CB	2.10	1.28
2:D:3072:SER:C	2:D:3073:ALA:N	2.02	1.16
1:C:2364:LYS:HE3	1:C:2365:THR:CG2	2.02	0.89
1:A:447:GLN:HG3	6:A:2489:HOH:O	1.82	0.80
1:C:2364:LYS:HE3	1:C:2365:THR:HG22	1.64	0.80
1:C:2117:ASP:CB	1:C:2117:ASP:OD2	2.36	0.73
1:C:2364:LYS:HE3	1:C:2365:THR:HG23	1.69	0.72
2:D:3072:SER:O	2:D:3073:ALA:N	2.28	0.66
1:C:2117:ASP:CG	1:C:2117:ASP:CA	2.68	0.64
1:A:6:GLU:HG2	6:A:2007:HOH:O	1.99	0.61
1:A:215:ILE:CD1	1:A:215:ILE:HB	2.27	0.60
1:A:215:ILE:CB	1:A:215:ILE:HD12	2.26	0.59
6:C:4456:HOH:O	2:D:3032:HIS:HD2	1.87	0.57
1:C:2181:ARG:H	2:D:3040:GLN:HE22	1.51	0.57
6:A:2454:HOH:O	2:B:1032:HIS:HD2	1.88	0.57
1:C:2114:TRP:HH2	1:C:2117:ASP:CG	2.13	0.56
1:A:3:LYS:HE2	1:A:7:LEU:HG	1.88	0.55
1:C:2296:LYS:NZ	1:C:2328:HIS:HE1	2.05	0.55
2:D:3072:SER:CA	2:D:3073:ALA:N	2.72	0.52
1:A:464:ASP:HB3	6:A:2504:HOH:O	2.08	0.52
1:C:2114:TRP:HH2	1:C:2117:ASP:OD1	1.92	0.52
1:C:2114:TRP:CZ3	1:C:2116:GLY:HA2	2.45	0.52
1:A:394:ASN:HD22	1:A:395:GLN:H	1.57	0.52
2:B:1073:ALA:N	6:B:2133:HOH:O	2.43	0.52
1:A:424:PRO:HD3	6:A:2453:HOH:O	2.09	0.51
1:C:2117:ASP:OD2	1:C:2118:GLY:N	2.44	0.51
1:A:215:ILE:HG21	1:A:215:ILE:HD13	0.54	0.48
1:A:212:ASP:HB2	1:A:215:ILE:HD12	1.95	0.47
1:A:212:ASP:HB2	1:A:215:ILE:CD1	2.45	0.47
1:A:448:ASN:OD1	1:A:564:LYS:NZ	2.48	0.47
1:C:2114:TRP:CH2	1:C:2117:ASP:OD1	2.68	0.47
1:A:114:TRP:CZ3	1:A:116:GLY:HA2	2.50	0.46
2:B:1063:LYS:NZ	6:B:2121:HOH:O	2.48	0.46
2:B:1023:ILE:HD12	2:B:1030:PRO:HD3	1.98	0.45
6:A:2335:HOH:O	2:B:1032:HIS:HE1	2.00	0.44
4:A:1597:GOL:H32	1:C:2041:ARG:NH1	2.32	0.44
1:C:2114:TRP:CH2	1:C:2117:ASP:CG	2.95	0.44
1:A:447:GLN:NE2	6:A:2487:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3598:GOL:O3	4:C:3598:GOL:C2	2.56	0.44
1:C:2038:LYS:HD3	6:C:4543:HOH:O	2.18	0.43
1:A:296:LYS:NZ	1:A:328:HIS:HE1	2.16	0.43
1:C:2359:LYS:NZ	6:C:4397:HOH:O	2.51	0.42
1:A:466:LYS:NZ	6:A:2506:HOH:O	2.52	0.42
1:C:2553:THR:HG22	6:C:4473:HOH:O	2.19	0.42
6:C:4337:HOH:O	2:D:3032:HIS:HE1	2.03	0.41
1:C:2038:LYS:HE2	1:C:2038:LYS:HB2	1.84	0.41
1:A:62:ASP:HB3	6:A:2116:HOH:O	2.20	0.41
1:A:215:ILE:HB	1:A:215:ILE:HD12	2.00	0.40
1:A:68:HIS:CE1	1:A:110:GLY:HA2	2.57	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	594/599 (99%)	562 (95%)	32 (5%)	0	100	100
1	C	595/599 (99%)	568 (96%)	26 (4%)	1 (0%)	43	16
2	B	71/74 (96%)	71 (100%)	0	0	100	100
2	D	70/74 (95%)	70 (100%)	0	0	100	100
All	All	1330/1346 (99%)	1271 (96%)	58 (4%)	1 (0%)	48	17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2119	LYS

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	473/478 (99%)	464 (98%)	9 (2%)	50	13
1	C	471/478 (98%)	465 (99%)	6 (1%)	61	25
2	B	60/63 (95%)	57 (95%)	3 (5%)	22	2
2	D	56/63 (89%)	55 (98%)	1 (2%)	51	16
All	All	1060/1082 (98%)	1041 (98%)	19 (2%)	51	16

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	23	SER
1	A	205	LYS
1	A	215	ILE
1	A	345	LEU
1	A	394	ASN
1	A	395	GLN
1	A	446	ARG
1	A	533	ILE
2	B	1007	LYS
2	B	1031	LYS
2	B	1072	SER
1	C	2006	GLU
1	C	2023	SER
1	C	2117	ASP
1	C	2291	LYS
1	C	2364	LYS
1	C	2395	GLN
2	D	3027	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	25	ASN
1	A	74	ASN
1	A	149	ASN
1	A	242	ASN
1	A	328	HIS
1	A	349	ASN
1	A	367	GLN
1	A	394	ASN
1	A	395	GLN
2	B	1032	HIS
1	C	2025	ASN
1	C	2242	ASN
1	C	2328	HIS
1	C	2395	GLN
1	C	2448	ASN
1	C	2567	ASN
2	D	3032	HIS
2	D	3040	GLN

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	A	1596	5	26,26,26	4.83	13 (50%)	34,40,40	3.45	16 (47%)
4	GOL	A	1598	-	5,5,5	5.81	4 (80%)	5,5,5	2.38	1 (20%)
4	GOL	A	1597	-	5,5,5	4.86	4 (80%)	5,5,5	1.73	1 (20%)
3	PQQ	C	3597	5	26,26,26	3.81	18 (69%)	34,40,40	2.54	16 (47%)
4	GOL	C	3598	-	5,5,5	5.10	4 (80%)	5,5,5	2.15	1 (20%)

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	A	1596	5	-	0/12/28/28	0/3/3/3
4	GOL	A	1598	-	-	2/4/4/4	-
4	GOL	A	1597	-	-	1/4/4/4	-
3	PQQ	C	3597	5	-	1/12/28/28	0/3/3/3
4	GOL	C	3598	-	-	2/4/4/4	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1596	PQQ	C5-C4	-15.22	1.33	1.54
4	A	1598	GOL	O3-C3	8.76	1.79	1.42
3	A	1596	PQQ	O5-C5	8.59	1.41	1.23
4	C	3598	GOL	O3-C3	8.30	1.77	1.42
3	C	3597	PQQ	C6A-C5	8.21	1.60	1.50
3	A	1596	PQQ	C2-N1	7.97	1.51	1.37
4	A	1597	GOL	O3-C3	7.89	1.75	1.42
3	C	3597	PQQ	O5-C5	7.71	1.39	1.23
4	A	1598	GOL	O1-C1	-7.32	1.11	1.42
3	A	1596	PQQ	C9-C9A	7.06	1.51	1.41
3	C	3597	PQQ	C7-N6	6.54	1.44	1.34
3	A	1596	PQQ	C9A-C6A	6.50	1.51	1.41
3	A	1596	PQQ	C7-N6	6.23	1.43	1.34
3	C	3597	PQQ	C8-C9	5.95	1.49	1.39
3	C	3597	PQQ	C9A-C6A	5.84	1.50	1.41
4	C	3598	GOL	O1-C1	-5.69	1.18	1.42
4	A	1597	GOL	O1-C1	-5.63	1.18	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1598	GOL	O2-C2	-5.36	1.27	1.43
4	C	3598	GOL	O2-C2	-4.73	1.29	1.43
3	A	1596	PQQ	C3A-C1A	4.55	1.50	1.40
3	A	1596	PQQ	O4-C4	4.51	1.33	1.23
3	C	3597	PQQ	C2-N1	4.29	1.45	1.37
3	A	1596	PQQ	C8-C9	4.24	1.46	1.39
4	A	1597	GOL	O2-C2	-4.21	1.31	1.43
3	C	3597	PQQ	C2-C2X	4.06	1.58	1.48
3	C	3597	PQQ	C5-C4	-4.05	1.49	1.54
3	C	3597	PQQ	C8-C7	3.72	1.50	1.40
3	C	3597	PQQ	O4-C4	3.40	1.31	1.23
3	A	1596	PQQ	O9A-C9X	3.36	1.32	1.22
3	C	3597	PQQ	O7B-C7X	-3.25	1.20	1.30
4	A	1598	GOL	C3-C2	-3.13	1.39	1.51
3	A	1596	PQQ	C3-C2	2.98	1.45	1.38
3	C	3597	PQQ	O9A-C9X	2.92	1.31	1.22
3	C	3597	PQQ	O2A-C2X	-2.76	1.15	1.22
4	C	3598	GOL	C3-C2	-2.57	1.42	1.51
4	A	1597	GOL	C3-C2	-2.54	1.42	1.51
3	C	3597	PQQ	O9B-C9X	2.48	1.37	1.30
3	C	3597	PQQ	O2B-C2X	2.37	1.37	1.30
3	A	1596	PQQ	O7B-C7X	-2.35	1.23	1.30
3	C	3597	PQQ	C7-C7X	2.33	1.54	1.50
3	C	3597	PQQ	C9-C9X	2.32	1.54	1.49
3	C	3597	PQQ	C9A-C1A	-2.06	1.43	1.46
3	A	1596	PQQ	C6A-N6	2.02	1.38	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1596	PQQ	O5-C5-C6A	-11.08	109.09	121.76
3	A	1596	PQQ	O5-C5-C4	7.52	127.96	118.14
3	A	1596	PQQ	C9-C8-C7	6.81	125.52	119.93
3	C	3597	PQQ	C9-C8-C7	-5.76	115.21	119.93
3	A	1596	PQQ	C8-C9-C9A	-5.18	113.69	120.33
4	A	1598	GOL	O2-C2-C3	5.03	130.01	109.18
3	C	3597	PQQ	O7A-C7X-C7	-4.84	111.57	121.30
3	C	3597	PQQ	C5-C6A-N6	-4.54	107.48	115.06
3	A	1596	PQQ	C3A-C3-C2	-4.50	103.31	107.94
3	C	3597	PQQ	C8-C9-C9A	4.28	125.82	120.33
4	C	3598	GOL	O2-C2-C3	4.15	126.36	109.18
3	A	1596	PQQ	C8-C7-C7X	4.01	128.50	119.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3597	PQQ	C8-C9-C9X	-3.87	107.03	117.89
3	A	1596	PQQ	C3-C3A-C1A	3.73	112.94	107.09
3	A	1596	PQQ	C6A-N6-C7	3.64	122.79	118.01
3	C	3597	PQQ	C1A-C3A-C4	-3.58	119.32	122.33
3	A	1596	PQQ	O9A-C9X-C9	-3.52	113.58	121.97
4	A	1597	GOL	O2-C2-C3	3.48	123.60	109.18
3	C	3597	PQQ	O5-C5-C4	3.41	122.59	118.14
3	C	3597	PQQ	O2B-C2X-C2	-3.31	107.13	114.27
3	A	1596	PQQ	C8-C7-N6	-3.28	117.72	123.41
3	A	1596	PQQ	C9A-C9-C9X	3.11	128.31	121.49
3	A	1596	PQQ	C3A-C4-C5	3.09	120.53	117.03
3	C	3597	PQQ	C9A-C6A-N6	3.01	127.94	123.58
3	C	3597	PQQ	O7B-C7X-C7	2.91	121.61	114.71
3	A	1596	PQQ	C1A-C3A-C4	-2.68	120.08	122.33
3	A	1596	PQQ	C9A-C6A-N6	-2.67	119.71	123.58
3	C	3597	PQQ	O2B-C2X-O2A	2.66	130.24	123.90
3	A	1596	PQQ	O7A-C7X-C7	-2.59	116.09	121.30
3	C	3597	PQQ	C3A-C4-C5	2.51	119.88	117.03
3	C	3597	PQQ	O9B-C9X-C9	2.39	122.08	115.28
3	C	3597	PQQ	O9B-C9X-O9A	-2.36	118.28	123.35
3	C	3597	PQQ	C8-C7-N6	-2.33	119.35	123.41
3	A	1596	PQQ	O9B-C9X-C9	2.26	121.71	115.28
3	C	3597	PQQ	C9A-C9-C9X	2.20	126.31	121.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1598	GOL	O1-C1-C2-C3
4	C	3598	GOL	C1-C2-C3-O3
4	A	1598	GOL	O2-C2-C3-O3
4	A	1597	GOL	O1-C1-C2-O2
4	C	3598	GOL	O1-C1-C2-O2
3	C	3597	PQQ	C3-C2-C2X-O2B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

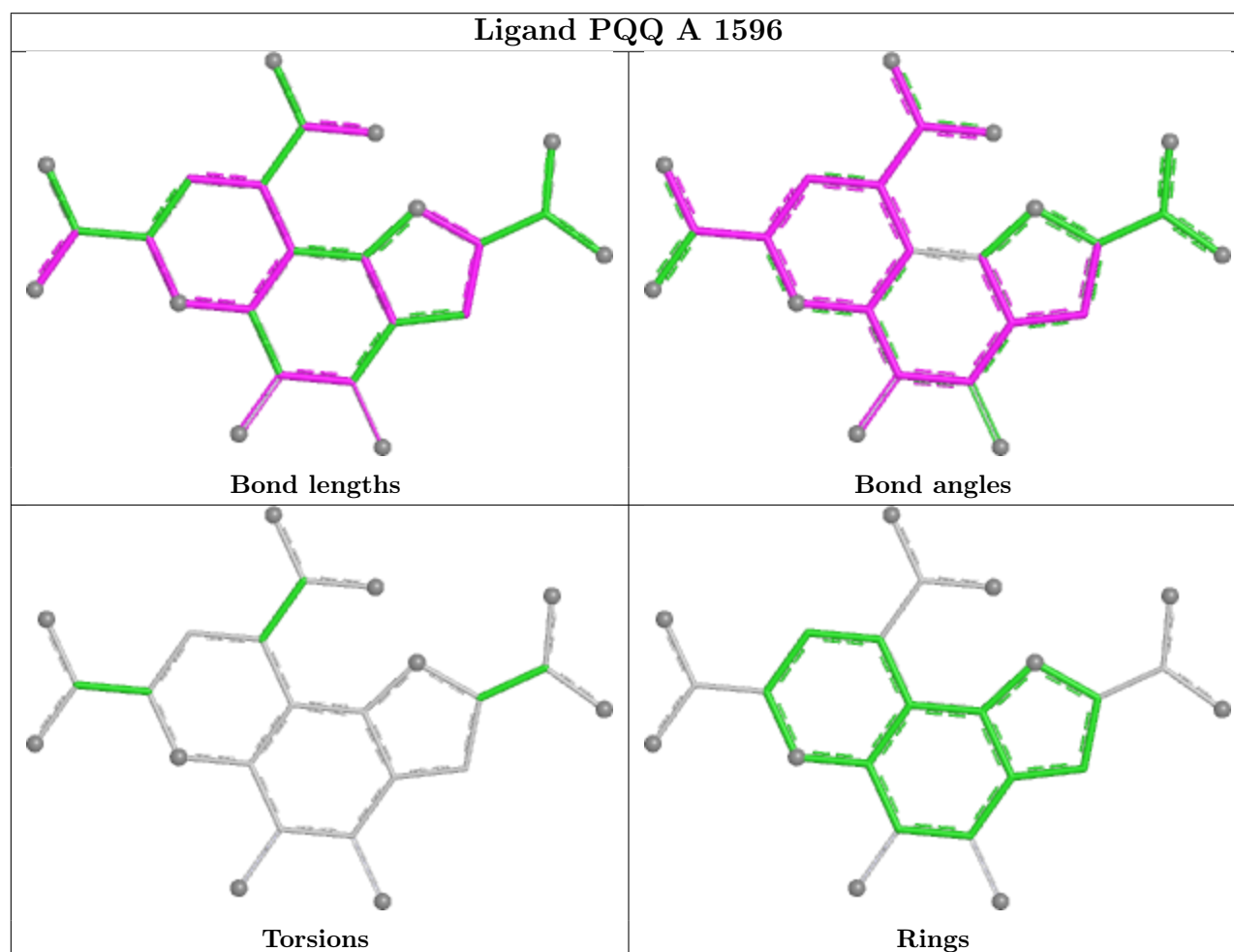
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1598	GOL	1	0
4	A	1597	GOL	2	0

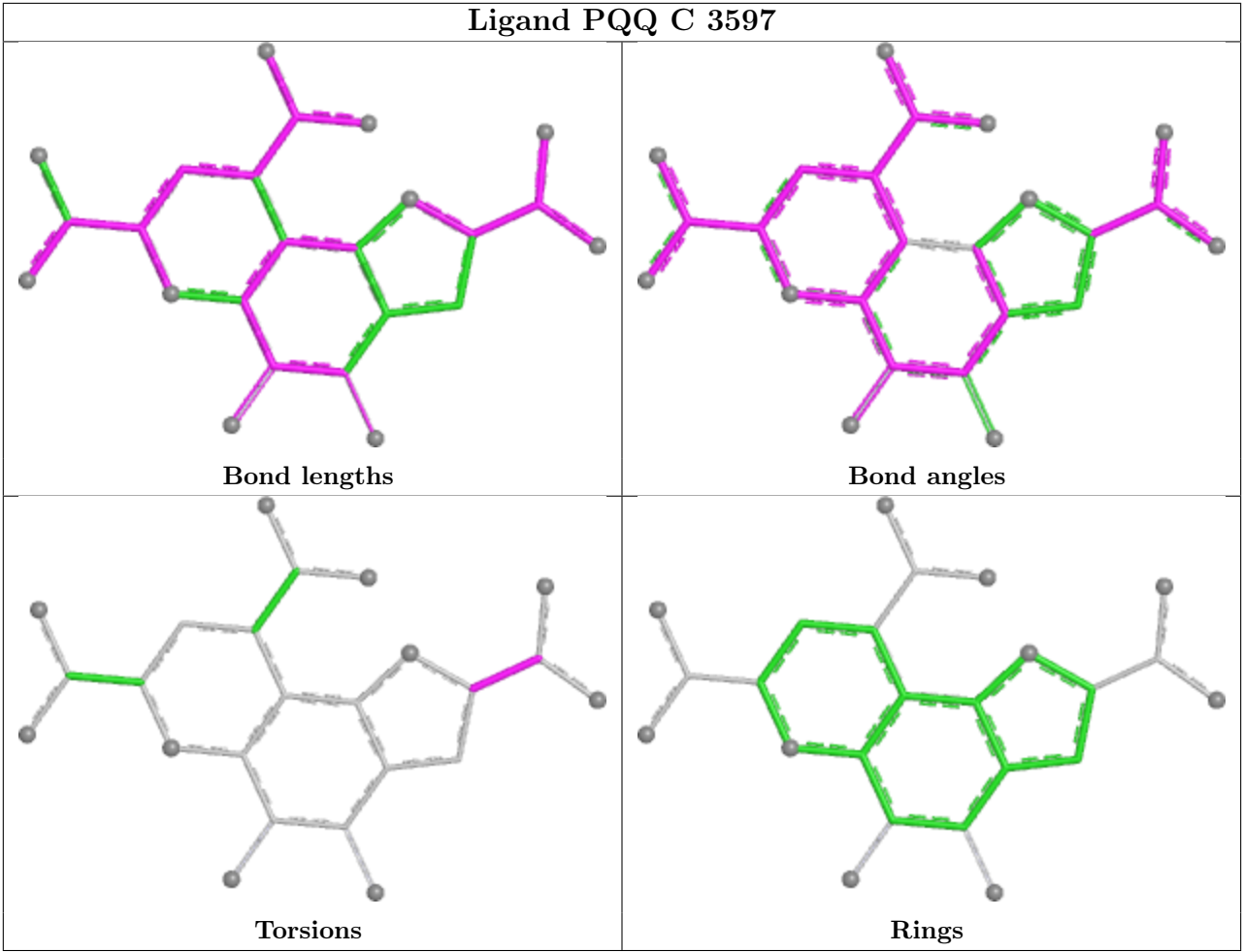
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3598	GOL	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3072:SER	C	3073:ALA	N	2.02

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	596/599 (99%)	-0.38	4 (0%) 84 87	9, 13, 26, 43	0
1	C	597/599 (99%)	-0.33	9 (1%) 72 73	9, 14, 26, 76	0
2	B	73/74 (98%)	-0.12	2 (2%) 56 55	12, 20, 33, 58	0
2	D	73/74 (98%)	0.06	2 (2%) 56 55	14, 24, 45, 78	0
All	All	1339/1346 (99%)	-0.32	17 (1%) 75 76	9, 14, 30, 78	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2118	GLY	6.2
2	B	1073	ALA	6.1
1	A	447	GLN	4.3
1	C	2597	ALA	4.3
1	C	2117	ASP	3.8
1	C	2596	SER	3.7
1	A	215	ILE	3.6
1	C	2364	LYS	3.5
1	C	2116	GLY	2.8
1	A	118	GLY	2.7
2	D	3073	ALA	2.6
2	B	1072	SER	2.5
1	C	2104	CYS	2.5
2	D	3068	VAL	2.5
1	C	2119	LYS	2.3
1	C	2120	THR	2.2
1	A	104	CYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

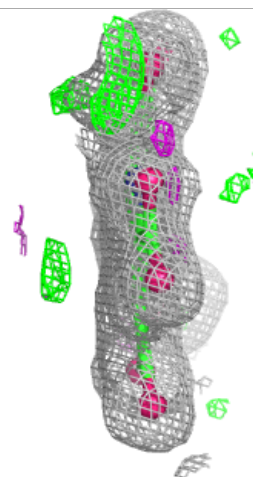
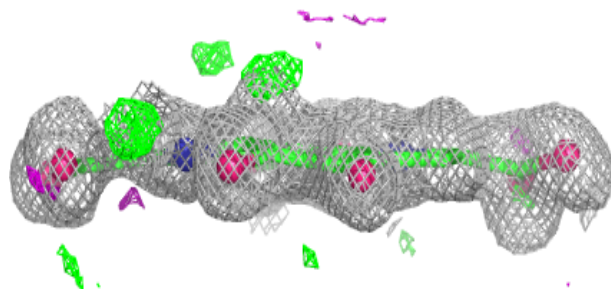
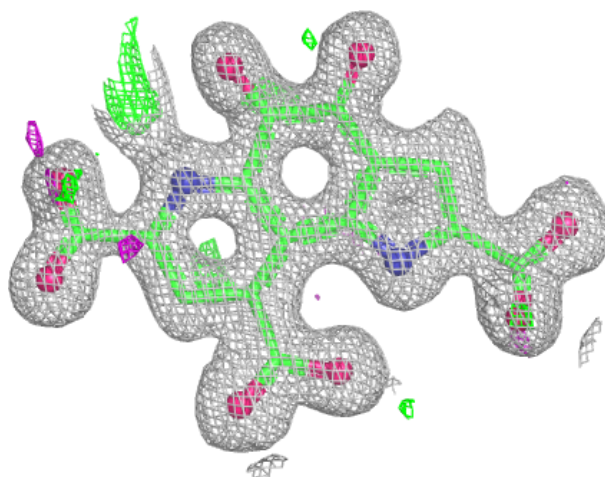
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

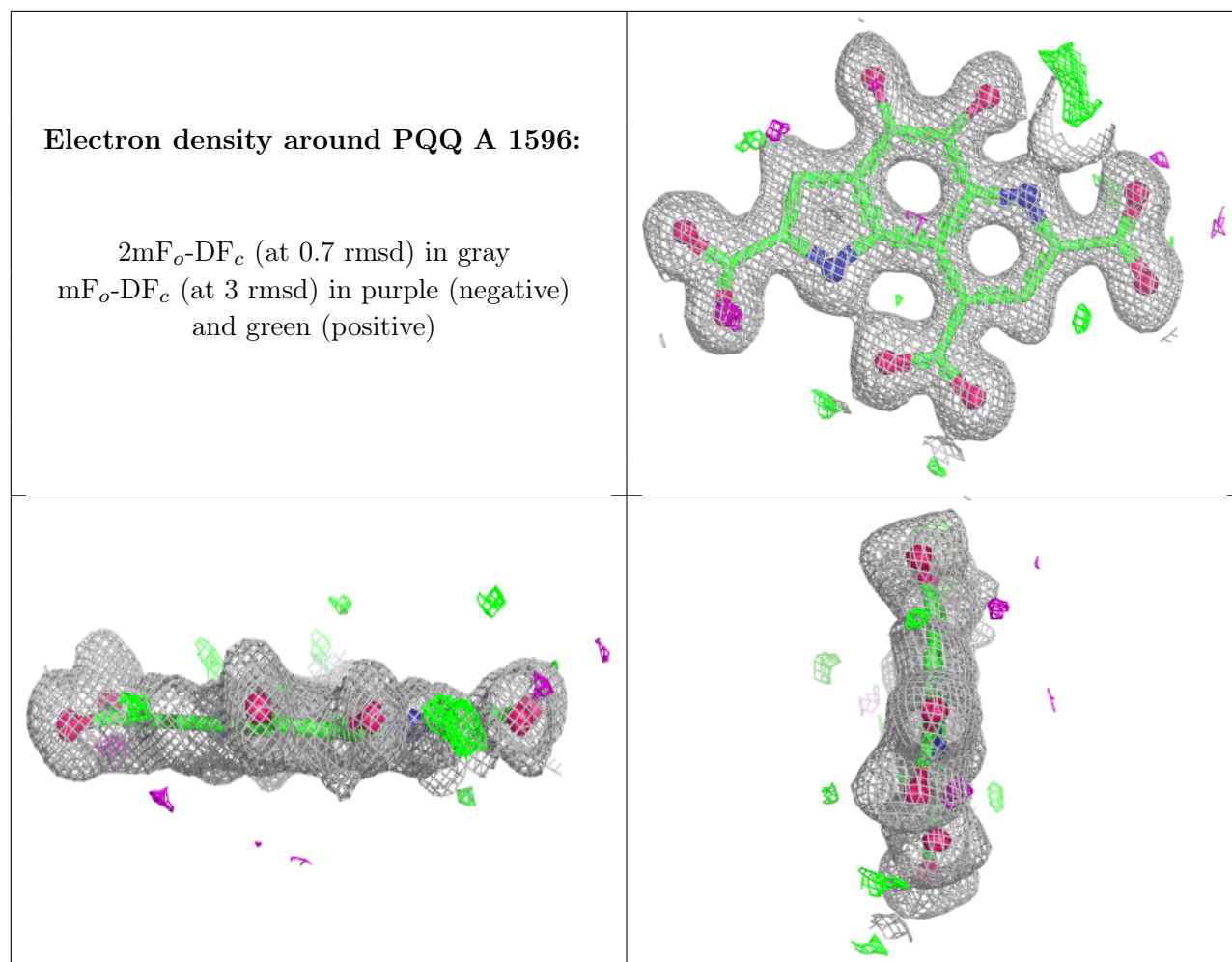
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	3598	6/6	0.93	0.09	14,17,18,22	0
4	GOL	A	1598	6/6	0.96	0.08	17,27,34,45	0
4	GOL	A	1597	6/6	0.96	0.07	12,17,19,20	0
3	PQQ	C	3597	24/24	0.97	0.04	11,15,19,21	0
3	PQQ	A	1596	24/24	0.98	0.04	12,14,19,21	0
5	CA	A	1599	1/1	0.99	0.07	25,25,25,25	1
5	CA	C	3599	1/1	1.00	0.09	25,25,25,25	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PQQ C 3597:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.