



# wwPDB X-ray Structure Validation Summary Report

Oct 15, 2014 – 07:22 PM EDT

PDB ID : 4TQO  
Title : The crystal structure of methanol dehydrogenase from *Methylococcus capsulatus* (Bath)  
Authors : Culpepper, M.A.; Rosenzweig, A.C.  
Deposited on : 2014-06-11  
Resolution : 2.57 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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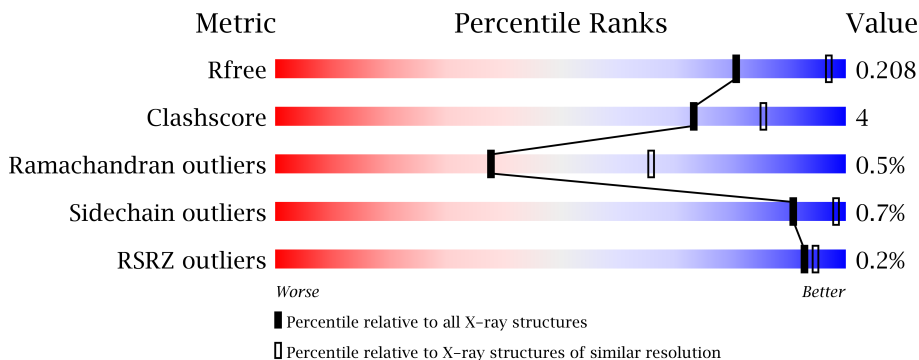
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23828
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.57 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))
$R_{free}$	66092	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	573	<div><div></div><div></div></div>
1	B	573	<div><div></div><div></div></div>
1	C	573	<div><div></div><div></div></div>
1	D	573	<div><div></div><div></div></div>
1	E	573	<div><div></div><div></div></div>
1	F	573	<div><div></div><div></div></div>
1	G	573	<div><div></div><div></div></div>
1	H	573	<div><div></div><div></div></div>
2	I	72	<div><div></div><div></div></div>
2	J	72	<div><div></div><div></div></div>
2	K	72	<div><div></div><div></div></div>
2	L	72	<div><div></div><div></div></div>
2	M	72	<div><div></div><div></div></div>
2	N	72	<div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	O	72	
2	P	72	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	PQQ	A	702	-	X
4	PQQ	B	702	-	X
4	PQQ	C	702	-	X
4	PQQ	D	702	-	X
4	PQQ	E	702	-	X
4	PQQ	F	702	-	X
4	PQQ	G	702	-	X
4	PQQ	H	702	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43059 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methanol dehydrogenase protein, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	A	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	C	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	D	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			
1	E	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	F	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	G	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	H	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			

- Molecule 2 is a protein called Methanol dehydrogenase, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	J	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	K	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	L	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	M	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			
2	N	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			

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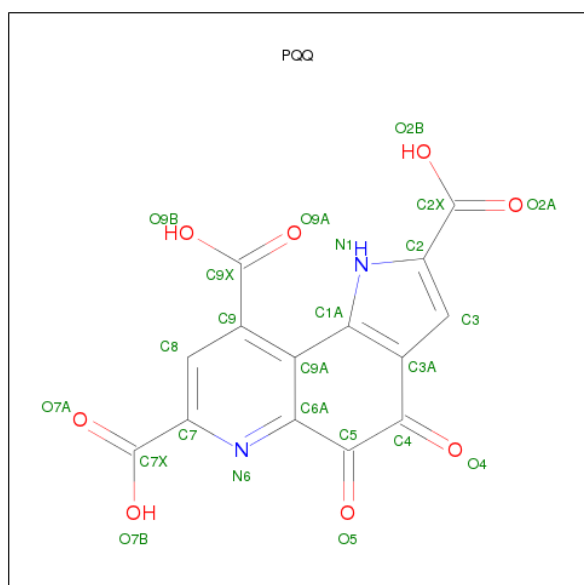
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			
2	P	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: C<sub>14</sub>H<sub>6</sub>N<sub>2</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			24	14	2	8		
4	A	1	Total	C	N	O	0	0
			24	14	2	8		
4	C	1	Total	C	N	O	0	0
			24	14	2	8		
4	D	1	Total	C	N	O	0	0
			24	14	2	8		
4	E	1	Total	C	N	O	0	0
			24	14	2	8		
4	F	1	Total	C	N	O	0	0
			24	14	2	8		
4	G	1	Total	C	N	O	0	0
			24	14	2	8		
4	H	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	276	Total	O	0	0
			276	276		
5	I	57	Total	O	0	0
			57	57		
5	A	288	Total	O	0	0
			288	288		
5	J	45	Total	O	0	0
			45	45		
5	C	237	Total	O	0	0
			237	237		
5	K	29	Total	O	0	0
			29	29		
5	D	247	Total	O	0	0
			247	247		
5	L	46	Total	O	0	0
			46	46		
5	E	241	Total	O	0	0
			241	241		
5	M	33	Total	O	0	0
			33	33		
5	F	251	Total	O	0	0
			251	251		
5	N	39	Total	O	0	0
			39	39		

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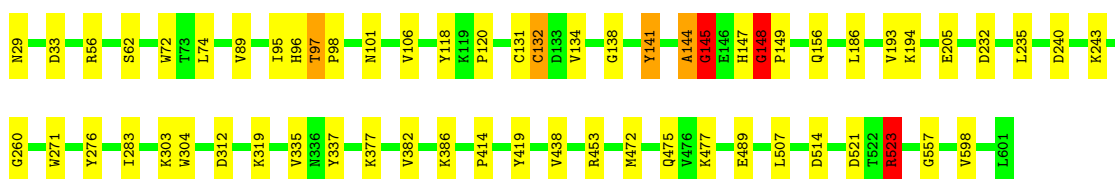
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	244	Total 244	O 244	0	0
5	O	35	Total 35	O 35	0	0
5	H	254	Total 254	O 254	0	0
5	P	30	Total 30	O 30	0	0

### 3 Residue-property plots

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

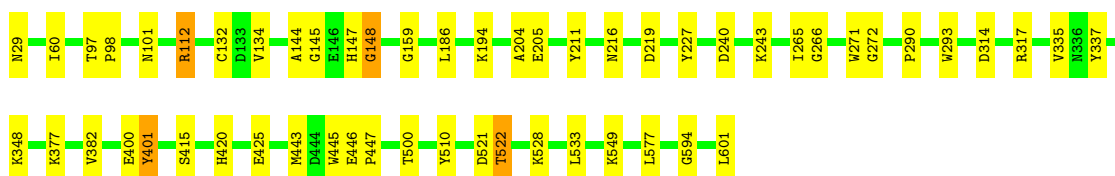
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain B: 



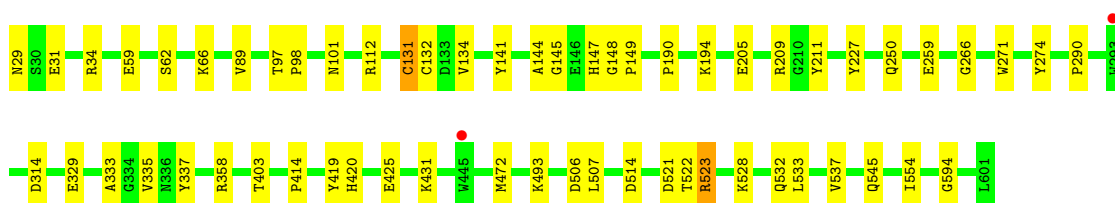
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain A: 



- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain C: 



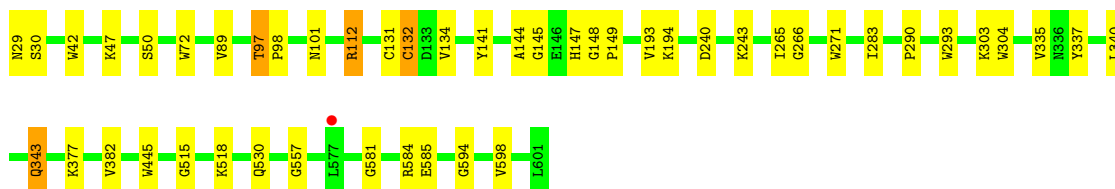
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain D: 



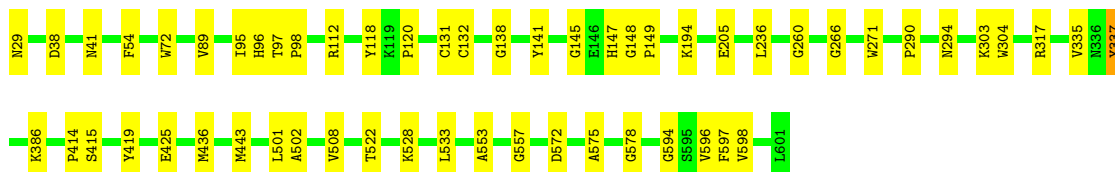
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain E:



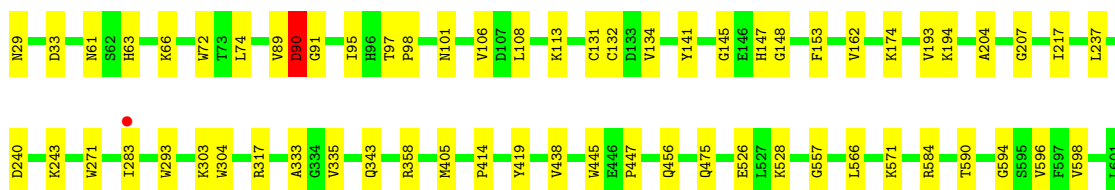
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain F:



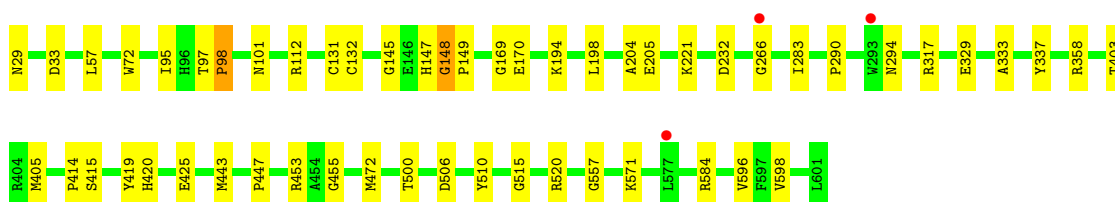
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain G:



- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain H:



- Molecule 2: Methanol dehydrogenase, small subunit

Chain I:



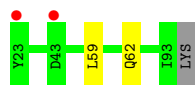
- Molecule 2: Methanol dehydrogenase, small subunit

Chain J:



- Molecule 2: Methanol dehydrogenase, small subunit

Chain K: 



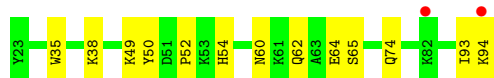
- Molecule 2: Methanol dehydrogenase, small subunit

Chain L: 



- Molecule 2: Methanol dehydrogenase, small subunit

Chain M: 



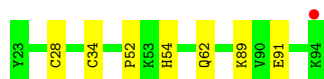
- Molecule 2: Methanol dehydrogenase, small subunit

Chain N: 



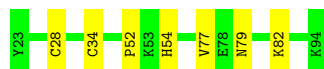
- Molecule 2: Methanol dehydrogenase, small subunit

Chain O: 



- Molecule 2: Methanol dehydrogenase, small subunit

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.49Å 210.29Å 231.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.15 – 2.57 105.14 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.9 (105.15-2.57) 100.0 (105.14-2.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, $R_{free}$	0.158 , 0.208 0.157 , 0.208	Depositor DCC
$R_{free}$ test set	9925 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 25.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 199002 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	43059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.37	2/4622 (0.0%)	0.49	0/6281
1	B	0.42	3/4622 (0.1%)	0.52	4/6281 (0.1%)
1	C	0.30	0/4622	0.47	0/6281
1	D	0.34	0/4621	0.49	0/6281
1	E	0.29	0/4622	0.48	0/6281
1	F	0.37	2/4622 (0.0%)	0.48	0/6281
1	G	0.27	0/4622	0.48	0/6281
1	H	0.28	0/4622	0.48	0/6281
2	I	0.34	0/583	0.42	0/785
2	J	0.28	0/583	0.43	0/785
2	K	0.25	0/583	0.41	0/785
2	L	0.27	0/583	0.42	0/785
2	M	0.31	0/592	0.54	0/796
2	N	0.33	0/592	0.53	1/796 (0.1%)
2	O	0.25	0/592	0.41	0/796
2	P	0.26	0/592	0.41	0/796
All	All	0.33	7/41675 (0.0%)	0.48	5/56572 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	TYR	CD1-CE1	-6.59	1.29	1.39
1	B	141	TYR	CD2-CE2	-5.91	1.30	1.39
1	A	401	TYR	CD2-CE2	-5.77	1.30	1.39
1	A	401	TYR	CD1-CE1	-5.66	1.30	1.39
1	B	148	GLY	C-O	-5.50	1.14	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	523	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	523	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	N	74	GLN	CA-CB-CG	6.28	127.21	113.40
1	B	144	ALA	C-N-CA	-5.72	110.28	122.30
1	B	145	GLY	N-CA-C	5.25	126.21	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4491	0	4320	47	0
1	B	4491	0	4320	40	0
1	C	4491	0	4320	38	0
1	D	4490	0	4320	31	0
1	E	4491	0	4320	31	0
1	F	4491	0	4320	37	0
1	G	4491	0	4320	42	0
1	H	4491	0	4320	36	0
2	I	568	0	545	6	0
2	J	568	0	545	3	0
2	K	568	0	545	2	0
2	L	568	0	545	3	0
2	M	577	0	558	12	0
2	N	577	0	558	9	0
2	O	577	0	558	5	0
2	P	577	0	558	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
4	A	24	0	3	3	0
4	B	24	0	3	3	0
4	C	24	0	3	1	0
4	D	24	0	3	1	0
4	E	24	0	3	0	0
4	F	24	0	3	2	0
4	G	24	0	3	2	0
4	H	24	0	3	2	0
5	A	288	0	0	3	0
5	B	276	0	0	5	1
5	C	237	0	0	9	0
5	D	247	0	0	7	1
5	E	241	0	0	3	0
5	F	251	0	0	8	0
5	G	244	0	0	9	0
5	H	254	0	0	9	1
5	I	57	0	0	3	1
5	J	45	0	0	1	1
5	K	29	0	0	1	0
5	L	46	0	0	2	0
5	M	33	0	0	3	0
5	N	39	0	0	2	1
5	O	35	0	0	0	0
5	P	30	0	0	0	0
All	All	43059	0	38996	337	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:400:GLU:OE1	1:A:401:TYR:CE2	1.71	1.41
1:A:400:GLU:OE1	1:A:401:TYR:CZ	1.79	1.33
1:A:400:GLU:OE1	1:A:401:TYR:CD2	2.09	1.03
2:M:35:TRP:O	5:M:706:HOH:O	1.80	0.98
1:A:400:GLU:OE1	1:A:401:TYR:CE1	2.26	0.89

All (3) 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	Distance(Å)	Clash(Å)
5:I:705:HOH:O	5:J:702:HOH:O[4_444]	2.00	0.20
5:B:811:HOH:O	5:H:810:HOH:O[3_554]	2.04	0.16
5:D:810:HOH:O	5:N:707:HOH:O[3_654]	2.10	0.10

## 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	571/573 (100%)	543 (95%)	25 (4%)	3 (0%)	38	66
1	B	571/573 (100%)	539 (94%)	28 (5%)	4 (1%)	30	56
1	C	571/573 (100%)	537 (94%)	32 (6%)	2 (0%)	43	70
1	D	571/573 (100%)	536 (94%)	33 (6%)	2 (0%)	43	70
1	E	571/573 (100%)	541 (95%)	27 (5%)	3 (0%)	38	66
1	F	571/573 (100%)	533 (93%)	35 (6%)	3 (0%)	38	66
1	G	571/573 (100%)	538 (94%)	29 (5%)	4 (1%)	30	56
1	H	571/573 (100%)	536 (94%)	31 (5%)	4 (1%)	30	56
2	I	69/72 (96%)	69 (100%)	0	0	100	100
2	J	69/72 (96%)	69 (100%)	0	0	100	100
2	K	69/72 (96%)	69 (100%)	0	0	100	100
2	L	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	M	70/72 (97%)	70 (100%)	0	0	100	100
2	N	70/72 (97%)	68 (97%)	2 (3%)	0	100	100
2	O	70/72 (97%)	70 (100%)	0	0	100	100
2	P	70/72 (97%)	70 (100%)	0	0	100	100
All	All	5124/5160 (99%)	4856 (95%)	243 (5%)	25 (0%)	38	66

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	GLY
1	D	294	ASN
1	G	90	ASP
1	H	294	ASN
1	F	294	ASN

### 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	464/464 (100%)	461 (99%)	3 (1%)	92	98
1	B	464/464 (100%)	458 (99%)	6 (1%)	80	94
1	C	464/464 (100%)	459 (99%)	5 (1%)	84	96
1	D	464/464 (100%)	460 (99%)	4 (1%)	87	97
1	E	464/464 (100%)	459 (99%)	5 (1%)	84	96
1	F	464/464 (100%)	463 (100%)	1 (0%)	96	99
1	G	464/464 (100%)	463 (100%)	1 (0%)	96	99
1	H	464/464 (100%)	461 (99%)	3 (1%)	92	98
2	I	60/61 (98%)	60 (100%)	0	100	100
2	J	60/61 (98%)	60 (100%)	0	100	100
2	K	60/61 (98%)	60 (100%)	0	100	100
2	L	60/61 (98%)	60 (100%)	0	100	100
2	M	61/61 (100%)	61 (100%)	0	100	100
2	N	61/61 (100%)	61 (100%)	0	100	100
2	O	61/61 (100%)	61 (100%)	0	100	100
2	P	61/61 (100%)	61 (100%)	0	100	100
All	All	4196/4200 (100%)	4168 (99%)	28 (1%)	91	98

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	522	THR
1	D	97	THR

*Continued on next page...*

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Mol	Chain	Res	Type
1	H	170	GLU
1	C	523	ARG
1	D	53	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	74	GLN
1	G	63	HIS
2	N	74	GLN
2	I	79	ASN
2	N	79	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z  > 2$
4	PQQ	A	702	-	26,26,26	1.03	1 (3%)	39,40,40	2.41	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PQQ	B	702	-	26,26,26	1.06	1 (3%)	39,40,40	2.47	7 (17%)
4	PQQ	C	702	-	26,26,26	1.09	1 (3%)	39,40,40	2.30	6 (15%)
4	PQQ	D	702	-	26,26,26	1.15	1 (3%)	39,40,40	2.43	5 (12%)
4	PQQ	E	702	-	26,26,26	1.05	1 (3%)	39,40,40	2.56	6 (15%)
4	PQQ	F	702	-	26,26,26	1.03	1 (3%)	39,40,40	2.60	7 (17%)
4	PQQ	G	702	-	26,26,26	1.06	1 (3%)	39,40,40	2.42	5 (12%)
4	PQQ	H	702	-	26,26,26	1.06	1 (3%)	39,40,40	2.64	3 (7%)

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
4	PQQ	A	702	-	-	1/10/28/28	0/3/3/3
4	PQQ	B	702	-	-	0/10/28/28	0/3/3/3
4	PQQ	C	702	-	-	1/10/28/28	0/3/3/3
4	PQQ	D	702	-	-	1/10/28/28	0/3/3/3
4	PQQ	E	702	-	-	1/10/28/28	0/3/3/3
4	PQQ	F	702	-	-	1/10/28/28	0/3/3/3
4	PQQ	G	702	-	-	0/10/28/28	0/3/3/3
4	PQQ	H	702	-	-	1/10/28/28	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	702	PQQ	C5-C4	-3.17	1.44	1.53
4	F	702	PQQ	C5-C4	-3.12	1.44	1.53
4	C	702	PQQ	C5-C4	-3.11	1.44	1.53
4	A	702	PQQ	C5-C4	-3.04	1.44	1.53
4	E	702	PQQ	C5-C4	-3.04	1.44	1.53

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	702	PQQ	C2X-C2-N1	14.54	128.07	116.85
4	E	702	PQQ	C2X-C2-N1	13.77	127.47	116.85
4	F	702	PQQ	C2X-C2-N1	13.63	127.37	116.85
4	D	702	PQQ	C2X-C2-N1	12.93	126.83	116.85
4	G	702	PQQ	C2X-C2-N1	12.55	126.53	116.85

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	702	PQQ	O2A-C2X-C2-N1
4	F	702	PQQ	O2A-C2X-C2-N1
4	C	702	PQQ	O2A-C2X-C2-N1
4	D	702	PQQ	O2A-C2X-C2-N1
4	H	702	PQQ	O2A-C2X-C2-N1

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	573/573 (100%)	-0.31	0 100 100	15, 21, 32, 46	0
1	B	573/573 (100%)	-0.38	0 100 100	15, 22, 33, 49	0
1	C	573/573 (100%)	-0.17	2 (0%) 91 93	15, 25, 36, 53	0
1	D	573/573 (100%)	-0.36	0 100 100	16, 23, 34, 50	0
1	E	573/573 (100%)	-0.35	1 (0%) 93 95	16, 23, 35, 48	0
1	F	573/573 (100%)	-0.39	0 100 100	15, 24, 34, 45	0
1	G	573/573 (100%)	-0.33	1 (0%) 93 95	15, 24, 35, 50	0
1	H	573/573 (100%)	-0.21	3 (0%) 88 90	16, 24, 36, 52	0
2	I	71/72 (98%)	-0.21	0 100 100	21, 27, 45, 53	0
2	J	71/72 (98%)	-0.19	0 100 100	22, 27, 41, 48	0
2	K	71/72 (98%)	0.10	2 (2%) 50 49	28, 36, 46, 51	0
2	L	71/72 (98%)	-0.28	0 100 100	19, 31, 44, 55	0
2	M	72/72 (100%)	-0.09	2 (2%) 50 49	24, 31, 48, 64	0
2	N	72/72 (100%)	-0.30	0 100 100	25, 32, 44, 48	0
2	O	72/72 (100%)	-0.09	1 (1%) 72 73	25, 36, 48, 59	0
2	P	72/72 (100%)	0.18	0 100 100	23, 32, 47, 59	0
All	All	5156/5160 (99%)	-0.29	12 (0%) 93 95	15, 24, 38, 64	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	293	TRP	3.0
2	O	94	LYS	2.8
1	H	577	LEU	2.7
1	C	445	TRP	2.5
2	M	94	LYS	2.4

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PQQ	F	702	24/24	0.26	6.09	28,38,42,45	0
4	PQQ	B	702	24/24	0.24	5.97	27,36,40,43	0
4	PQQ	D	702	24/24	0.26	5.26	29,39,45,47	0
4	PQQ	G	702	24/24	0.27	4.80	25,38,43,44	0
4	PQQ	E	702	24/24	0.26	4.78	27,40,43,45	0
4	PQQ	H	702	24/24	0.33	4.21	30,42,48,50	0
4	PQQ	A	702	24/24	0.23	2.70	25,33,36,38	0
4	PQQ	C	702	24/24	0.22	2.07	26,36,42,44	0
3	CA	A	701	1/1	0.13	-0.89	40,40,40,40	0
3	CA	C	701	1/1	0.12	-1.00	46,46,46,46	0
3	CA	H	701	1/1	0.16	-1.32	97,97,97,97	0
3	CA	G	701	1/1	0.13	-2.01	43,43,43,43	0
3	CA	E	701	1/1	0.07	-2.36	39,39,39,39	0
3	CA	B	701	1/1	0.06	-3.28	37,37,37,37	0
3	CA	D	701	1/1	0.06	-3.31	44,44,44,44	0
3	CA	F	701	1/1	0.07	-3.55	49,49,49,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.