Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 04:09 PM EDT

PDB ID	:	4AAH
Title	:	METHANOL DEHYDROGENASE FROM METHYLOPHILUS W3A1
Authors	:	Mathews, F.S.; Xia, Z.-X.
Deposited on	:	1996-03-10
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

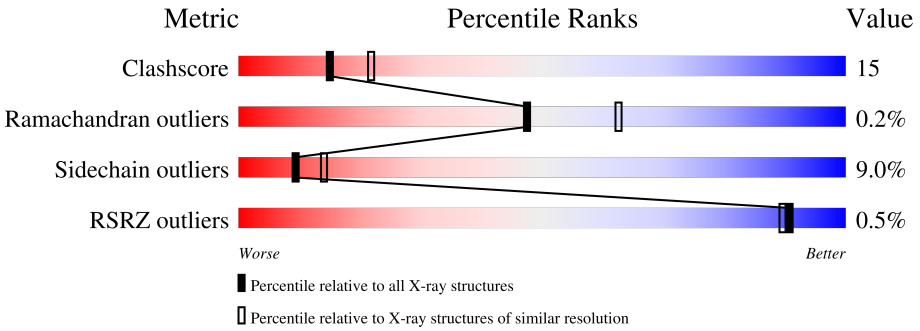
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	571	62% 31% 7% •
1	C	571	71% 23% 5% •
2	B	69	4% 51% 45% •
2	D	69	6% 68% 25% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10465 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	571	4402	2809	752	815	26	0	0	0
1	C	571	4402	2809	752	815	26	0	0	0

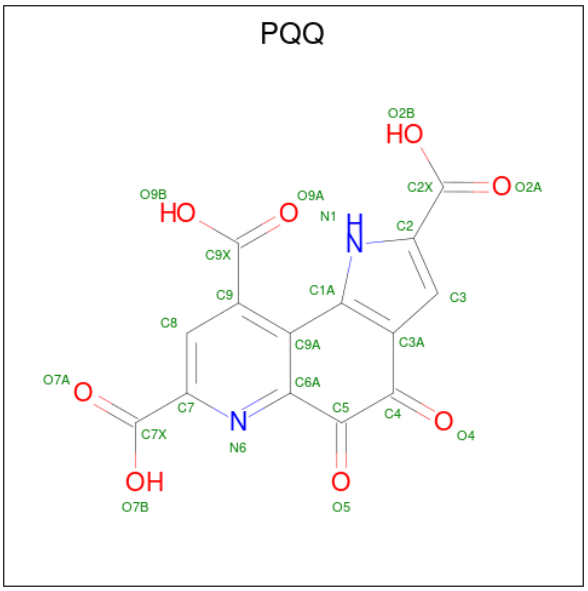
- Molecule 2 is a protein called METHANOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	69	545	337	97	108	3	0	0	0
2	D	69	545	337	97	108	3	0	0	0

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

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

- Molecule 4 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: $C_{14}H_6N_2O_8$).



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

- Molecule 5 is water.

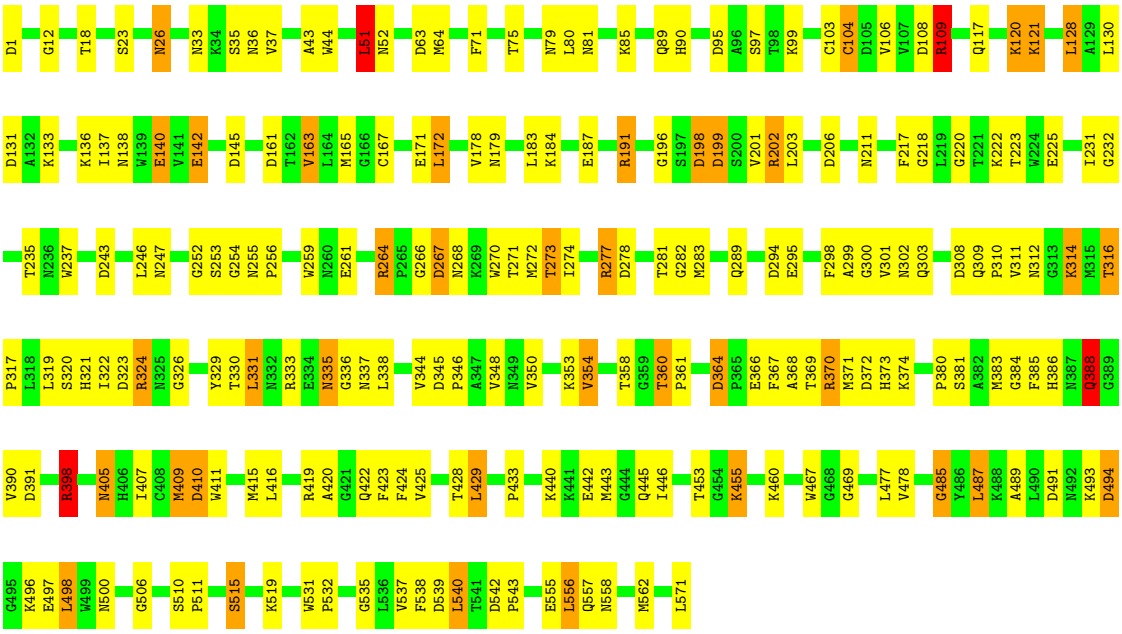
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	216	216	216	0	0
			Total	O		
5	B	15	15	15	0	0
			Total	O		
5	C	265	265	265	0	0
			Total	O		
5	D	25	25	25	0	0

3 Residue-property plots (i)

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

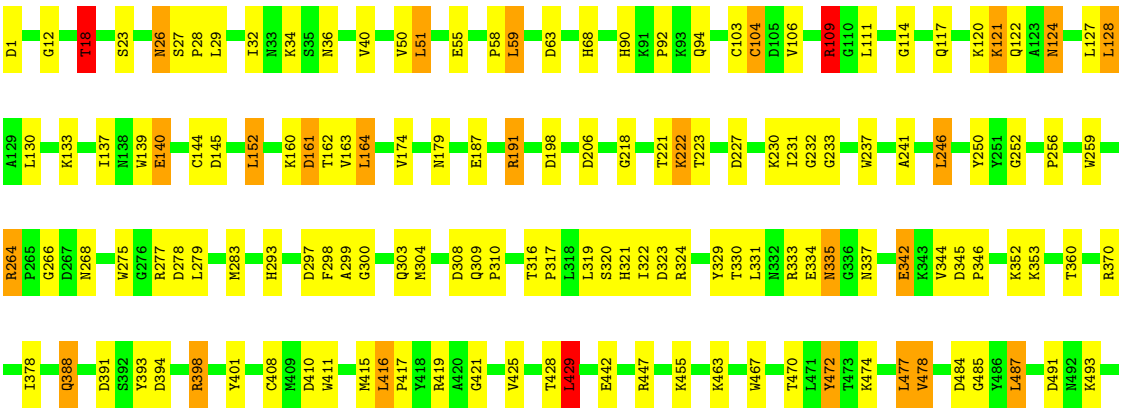
• Molecule 1: METHANOL DEHYDROGENASE

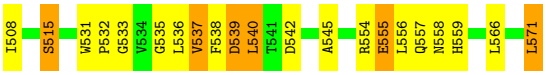
Chain A: 62% 31% 7% •



• Molecule 1: METHANOL DEHYDROGENASE

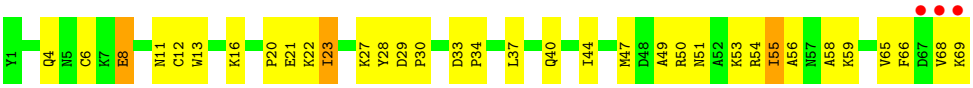
Chain C: 71% 23% 5% •





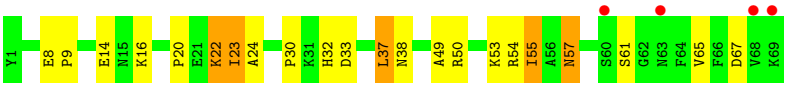
• Molecule 2: METHANOL DEHYDROGENASE

Chain B:



• Molecule 2: METHANOL DEHYDROGENASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.90Å 62.70Å 85.00Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 21.40 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (10.00-2.40) 93.2 (21.40-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.31Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.152 , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10465	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0821e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.94	0/4529	1.61	64/6150 (1.0%)
1	C	0.98	0/4529	1.61	51/6150 (0.8%)
2	B	0.82	0/557	1.46	2/746 (0.3%)
2	D	0.88	0/557	1.52	4/746 (0.5%)
All	All	0.95	0/10172	1.60	121/13792 (0.9%)

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	2
All	All	0	3

There are no bond length outliers.

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	333	ARG	NE-CZ-NH2	17.29	128.94	120.30
1	A	109	ARG	NE-CZ-NH1	-13.97	113.31	120.30
1	C	161	ASP	CB-CG-OD1	13.62	130.56	118.30
1	C	370	ARG	NE-CZ-NH1	13.16	126.88	120.30
1	A	398	ARG	CD-NE-CZ	13.11	141.96	123.60
1	A	324	ARG	NE-CZ-NH1	-12.24	114.18	120.30
1	A	202	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	C	398	ARG	NE-CZ-NH1	12.01	126.31	120.30
1	C	63	ASP	CB-CG-OD1	11.70	128.83	118.30
1	A	398	ARG	NE-CZ-NH1	11.60	126.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	ASP	CB-CG-OD1	11.54	128.68	118.30
1	A	109	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	A	131	ASP	CB-CG-OD1	10.60	127.84	118.30
1	C	333	ARG	NE-CZ-NH1	-10.43	115.09	120.30
2	D	54	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	A	202	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	C	410	ASP	CB-CG-OD2	-9.63	109.63	118.30
1	C	264	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	109	ARG	CD-NE-CZ	-9.13	110.82	123.60
1	A	145	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	A	308	ASP	CB-CG-OD1	8.80	126.22	118.30
1	C	419	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	C	227	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	333	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	308	ASP	CB-CG-OD2	-7.82	111.27	118.30
2	B	33	ASP	CB-CG-OD1	7.75	125.28	118.30
1	C	370	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	324	ARG	CD-NE-CZ	-7.70	112.83	123.60
1	A	283	MET	CA-CB-CG	7.56	126.15	113.30
1	A	199	ASP	CB-CG-OD1	7.32	124.89	118.30
1	C	447	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	485	GLY	N-CA-C	7.26	131.26	113.10
1	A	145	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	388	GLN	CA-CB-CG	7.21	129.27	113.40
1	A	370	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	485	GLY	N-CA-C	7.15	130.98	113.10
1	A	398	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	267	ASP	CB-CG-OD2	7.03	124.63	118.30
1	C	63	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	A	321	HIS	CA-CB-CG	6.99	125.47	113.60
1	C	393	TYR	CB-CG-CD1	6.86	125.12	121.00
1	A	198	ASP	CB-CG-OD1	6.86	124.47	118.30
1	C	198	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	264	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	C	410	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	63	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	241	ALA	N-CA-CB	6.61	119.36	110.10
1	C	308	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	128	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	161	ASP	CB-CG-OD1	6.56	124.20	118.30
1	C	477	LEU	CA-CB-CG	6.56	130.38	115.30
1	C	145	ASP	CB-CG-OD2	-6.50	112.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	472	TYR	CB-CG-CD2	-6.49	117.11	121.00
1	C	487	LEU	N-CA-C	-6.47	93.53	111.00
1	A	388	GLN	CB-CG-CD	6.44	128.35	111.60
1	A	354	VAL	CB-CA-C	6.41	123.57	111.40
1	C	104	CYS	N-CA-CB	-6.38	99.12	110.60
1	A	370	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	131	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	C	277	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	323	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	C	278	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	489	ALA	N-CA-CB	6.09	118.62	110.10
1	C	415	MET	O-C-N	6.05	132.38	122.70
1	A	131	ASP	CB-CA-C	5.99	122.38	110.40
1	A	494	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	283	MET	CA-CB-CG	-5.95	103.18	113.30
1	A	277	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	C	342	GLU	CB-CG-CD	5.89	130.11	114.20
1	A	277	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	C	297	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	A	206	ASP	CB-CG-OD2	5.82	123.53	118.30
1	C	484	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	333	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	104	CYS	N-CA-CB	-5.79	100.17	110.60
1	A	556	LEU	C-N-CA	5.77	136.13	121.70
1	C	264	ARG	CD-NE-CZ	5.76	131.67	123.60
1	C	109	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	C	227	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	364	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	C	161	ASP	OD1-CG-OD2	-5.71	112.45	123.30
1	C	1	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	1	ASP	CB-CG-OD1	5.67	123.41	118.30
1	C	323	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	35	SER	C-N-CA	5.63	135.78	121.70
1	C	140	GLU	CG-CD-OE2	5.61	129.52	118.30
2	D	33	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	50	VAL	CB-CA-C	5.54	121.92	111.40
1	A	1	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	95	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	D	50	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	A	191	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	A	253	SER	CB-CA-C	5.47	120.49	110.10
1	C	164	LEU	CA-CB-CG	5.47	127.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	VAL	CA-CB-CG1	5.44	119.06	110.90
1	A	51	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	410	ASP	N-CA-CB	5.43	120.38	110.60
1	C	333	ARG	CD-NE-CZ	-5.41	116.03	123.60
1	C	515	SER	CB-CA-C	-5.41	99.82	110.10
1	A	142	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	A	278	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	401	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	C	360	THR	CA-CB-CG2	5.35	119.89	112.40
1	A	409	MET	C-N-CA	5.28	134.91	121.70
1	C	18	THR	N-CA-CB	-5.26	100.31	110.30
1	A	487	LEU	N-CA-C	-5.22	96.91	111.00
1	A	225	GLU	CG-CD-OE1	5.21	128.71	118.30
1	C	555	GLU	OE1-CD-OE2	-5.20	117.07	123.30
1	C	139	TRP	CA-CB-CG	5.18	123.54	113.70
1	A	140	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	C	394	ASP	CB-CG-OD2	-5.15	113.66	118.30
2	D	14	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	A	274	ILE	O-C-N	5.12	130.90	122.70
1	A	446	ILE	N-CA-C	-5.09	97.26	111.00
1	C	429	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	393	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	198	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	460	LYS	CA-CB-CG	5.03	124.47	113.40
1	A	497	GLU	CG-CD-OE1	5.01	128.32	118.30
2	B	21	GLU	OE1-CD-OE2	5.00	129.31	123.30
1	C	152	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	C	109	ARG	Sidechain
1	C	191	ARG	Sidechain

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	4402	0	4250	155	0
1	C	4402	0	4250	113	0
2	B	545	0	522	31	0
2	D	545	0	522	15	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	24	0	3	3	0
4	C	24	0	3	3	0
5	A	216	0	0	9	0
5	B	15	0	0	1	0
5	C	265	0	0	6	0
5	D	25	0	0	1	0
All	All	10465	0	9550	295	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 15.

All (295) 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:187:GLU:HB2	2:B:55:ILE:HD13	1.38	1.01
1:A:117:GLN:HE21	1:A:138:ASN:ND2	1.64	0.94
1:C:90:HIS:HD2	1:C:120:LYS:HZ3	1.08	0.94
1:C:90:HIS:HD2	1:C:120:LYS:NZ	1.65	0.94
1:A:117:GLN:NE2	1:A:138:ASN:HD22	1.69	0.90
1:A:117:GLN:HE21	1:A:138:ASN:HD22	0.87	0.86
1:C:335:ASN:HD22	1:C:337:ASN:H	1.19	0.86
1:C:90:HIS:CD2	1:C:120:LYS:HZ3	1.93	0.85
1:C:309:GLN:HE21	1:C:398:ARG:HH11	1.24	0.81
1:A:64:MET:HE1	1:A:79:ASN:HB2	1.63	0.80
1:C:144:CYS:SG	1:C:152:LEU:HD13	2.21	0.80
1:A:311:VAL:HB	1:A:316:THR:HG21	1.62	0.80
1:A:64:MET:CE	1:A:79:ASN:HD22	1.94	0.79
1:C:18:THR:HG21	1:C:23:SER:OG	1.82	0.79
1:C:18:THR:CG2	1:C:23:SER:OG	2.30	0.79
2:B:51:ASN:ND2	2:B:54:ARG:HH21	1.80	0.78
1:C:179:ASN:ND2	1:C:191:ARG:HE	1.82	0.77
1:A:494:ASP:OD1	1:A:496:LYS:HG2	1.84	0.77
1:C:187:GLU:HB2	2:D:55:ILE:HD13	1.68	0.74
1:A:64:MET:HE2	1:A:79:ASN:HD22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:701:PQQ:N1	4:A:701:PQQ:O9B	2.23	0.72
1:A:319:LEU:C	1:A:319:LEU:HD23	2.08	0.71
1:A:335:ASN:C	1:A:335:ASN:HD22	1.94	0.71
1:A:142:GLU:OE2	2:B:54:ARG:NH2	2.19	0.71
1:A:485:GLY:HA2	1:A:506:GLY:HA2	1.73	0.70
1:A:136:LYS:HE3	5:A:907:HOH:O	1.90	0.70
1:C:26:ASN:HD22	1:C:26:ASN:C	1.95	0.70
1:A:273:THR:HG22	1:A:289:GLN:HG3	1.73	0.70
2:B:68:VAL:O	2:B:69:LYS:HB2	1.91	0.69
1:C:309:GLN:NE2	1:C:398:ARG:HH11	1.91	0.69
1:A:538:PHE:O	1:A:539:ASP:HB2	1.91	0.68
1:C:18:THR:HG23	1:C:23:SER:CB	2.24	0.67
1:C:40:VAL:HG22	1:C:571:LEU:HD13	1.76	0.67
1:A:538:PHE:HB2	1:A:540:LEU:HD22	1.77	0.66
1:A:324:ARG:HG3	1:A:386:HIS:O	1.95	0.66
1:A:335:ASN:HD22	1:A:336:GLY:N	1.92	0.66
1:C:335:ASN:ND2	1:C:337:ASN:H	1.92	0.66
2:D:53:LYS:O	2:D:57:ASN:HB2	1.96	0.66
1:A:311:VAL:HB	1:A:316:THR:CG2	2.26	0.65
1:C:128:LEU:HD23	1:C:128:LEU:N	2.11	0.65
1:C:218:GLY:O	1:C:222:LYS:HB2	1.95	0.65
1:A:428:THR:C	1:A:429:LEU:HD12	2.17	0.65
2:B:27:LYS:HE3	2:B:28:TYR:CZ	2.33	0.64
1:A:202:ARG:NH1	1:A:281:THR:O	2.30	0.64
1:A:538:PHE:HB2	1:A:540:LEU:CD2	2.28	0.63
1:A:259:TRP:CD2	1:A:425:VAL:HG13	2.33	0.63
1:C:68:HIS:HB2	5:C:723:HOH:O	1.99	0.62
1:A:270:TRP:O	1:A:273:THR:HG23	1.98	0.62
1:C:130:LEU:CD2	1:C:137:ILE:HG12	2.29	0.62
1:C:18:THR:HG23	1:C:23:SER:HA	1.81	0.62
1:A:386:HIS:NE2	1:A:391:ASP:OD2	2.28	0.62
1:C:319:LEU:HD23	1:C:319:LEU:C	2.21	0.61
1:C:303:GLN:HE22	1:C:391:ASP:H	1.47	0.61
1:C:174:VAL:O	1:C:233:GLY:HA2	2.00	0.61
1:C:55:GLU:HG3	1:C:508:ILE:HD12	1.83	0.61
1:A:26:ASN:HD22	1:A:26:ASN:C	2.04	0.61
1:C:378:ILE:O	1:C:408:CYS:HB3	2.00	0.60
1:A:429:LEU:HD12	1:A:429:LEU:N	2.17	0.60
1:C:18:THR:HG23	1:C:23:SER:OG	2.01	0.60
1:C:421:GLY:N	5:C:935:HOH:O	2.30	0.59
1:A:109:ARG:HE	1:A:388:GLN:HG3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:GLN:HG3	5:C:879:HOH:O	2.02	0.59
1:A:345:ASP:O	1:A:348:VAL:HG23	2.02	0.59
1:A:419:ARG:HB2	1:A:422:GLN:HG3	1.83	0.59
1:A:264:ARG:HH11	1:A:268:ASN:ND2	2.00	0.59
1:C:130:LEU:HD23	1:C:137:ILE:HG12	1.85	0.58
1:C:352:LYS:NZ	5:C:848:HOH:O	2.16	0.58
1:A:43:ALA:O	1:A:44:TRP:HB3	2.03	0.58
1:A:303:GLN:HE22	1:A:391:ASP:H	1.50	0.58
1:C:121:LYS:HB2	1:C:152:LEU:HD23	1.86	0.58
1:A:453:THR:OG1	1:A:455:LYS:HG3	2.04	0.57
1:A:109:ARG:HD3	1:A:388:GLN:HE21	1.69	0.57
1:A:109:ARG:CD	1:A:388:GLN:HE21	2.17	0.57
1:A:261:GLU:HG2	1:A:369:THR:O	2.04	0.57
1:A:542:ASP:OD1	1:A:543:PRO:HD2	2.04	0.57
2:D:20:PRO:HG2	2:D:23:ILE:HD12	1.87	0.57
1:C:32:ILE:HG12	1:C:571:LEU:HD22	1.86	0.56
1:A:335:ASN:ND2	1:A:337:ASN:H	2.03	0.56
1:C:160:LYS:HD3	1:C:279:LEU:HD23	1.87	0.56
1:C:335:ASN:HD21	1:C:337:ASN:HB2	1.71	0.56
1:C:246:LEU:HD21	1:C:334:GLU:CG	2.35	0.56
4:C:701:PQQ:O9B	4:C:701:PQQ:N1	2.39	0.56
1:A:537:VAL:HG22	1:A:562:MET:SD	2.46	0.56
1:A:117:GLN:NE2	5:A:794:HOH:O	2.39	0.55
1:A:531:TRP:N	1:A:532:PRO:CD	2.68	0.55
1:A:109:ARG:HE	1:A:388:GLN:CG	2.19	0.55
1:C:246:LEU:HD21	1:C:334:GLU:HG2	1.86	0.55
1:A:142:GLU:H	2:B:51:ASN:HD21	1.55	0.55
1:A:319:LEU:HD23	1:A:320:SER:N	2.21	0.55
1:A:535:GLY:HA2	1:A:540:LEU:HB2	1.89	0.55
1:C:179:ASN:HD22	1:C:191:ARG:HE	1.53	0.55
1:A:310:PRO:HA	1:A:314:LYS:O	2.07	0.55
2:B:51:ASN:HD22	2:B:54:ARG:HH21	1.50	0.55
1:A:277:ARG:HD3	1:A:282:GLY:O	2.07	0.55
1:C:470:THR:HB	1:C:478:VAL:HG23	1.89	0.55
1:A:64:MET:HE1	1:A:79:ASN:HD22	1.70	0.54
1:A:383:MET:HE3	1:A:467:TRP:CH2	2.42	0.54
1:A:557:GLN:OE1	1:A:558:ASN:ND2	2.41	0.54
1:C:55:GLU:HG3	1:C:508:ILE:CD1	2.38	0.54
1:C:109:ARG:HG3	1:C:109:ARG:NH1	2.22	0.54
1:A:142:GLU:OE1	2:B:50:ARG:NH1	2.41	0.54
1:A:360:THR:CG2	2:B:4:GLN:OE1	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:NH1	1:A:109:ARG:HG3	2.21	0.53
1:A:345:ASP:OD2	5:A:742:HOH:O	2.19	0.53
5:A:880:HOH:O	2:B:16:LYS:HD2	2.09	0.53
2:B:54:ARG:HD2	2:B:66:PHE:O	2.08	0.53
1:A:326:GLY:O	1:A:344:VAL:HG22	2.09	0.53
1:C:18:THR:HG23	1:C:23:SER:CA	2.38	0.53
1:A:433:PRO:HB3	1:A:443:MET:HG2	1.91	0.53
1:A:232:GLY:O	1:A:256:PRO:HA	2.09	0.53
1:A:237:TRP:CE2	1:A:301:VAL:HG21	2.44	0.53
1:A:142:GLU:HB2	2:B:47:MET:HG3	1.89	0.53
1:C:555:GLU:OE2	1:C:558:ASN:OD1	2.27	0.53
1:C:231:ILE:HD13	2:D:37:LEU:HD11	1.91	0.53
1:C:237:TRP:CZ2	4:C:701:PQQ:C6A	2.91	0.53
1:C:533:GLY:O	1:C:537:VAL:HG13	2.08	0.53
1:A:71:PHE:CE2	1:A:99:LYS:HD2	2.45	0.52
1:C:309:GLN:HB3	1:C:310:PRO:HD2	1.90	0.52
1:A:309:GLN:OE1	1:A:398:ARG:HG2	2.09	0.52
1:C:428:THR:C	1:C:429:LEU:HD12	2.30	0.52
1:C:103:CYS:SG	1:C:104:CYS:N	2.83	0.52
1:C:268:ASN:ND2	1:C:293:HIS:HA	2.25	0.52
1:A:103:CYS:SG	1:A:104:CYS:N	2.82	0.52
2:B:56:ALA:C	2:B:58:ALA:H	2.13	0.52
1:C:34:LYS:HD3	1:C:491:ASP:CG	2.30	0.52
2:B:66:PHE:O	2:B:68:VAL:N	2.39	0.52
2:D:23:ILE:HG23	2:D:30:PRO:HD3	1.92	0.52
1:C:127:LEU:C	1:C:128:LEU:HD23	2.30	0.51
1:C:92:PRO:HB3	1:C:122:GLN:NE2	2.26	0.51
1:C:94:GLN:HE21	1:C:124:ASN:HB3	1.76	0.51
2:B:8:GLU:HG3	2:B:11:ASN:HB3	1.94	0.50
1:A:271:THR:O	1:A:273:THR:CG2	2.60	0.50
1:A:64:MET:HE2	1:A:79:ASN:ND2	2.26	0.50
1:A:99:LYS:HG2	1:A:106:VAL:HG11	1.93	0.50
1:C:264:ARG:HH11	1:C:268:ASN:ND2	2.10	0.50
1:C:128:LEU:HD22	1:C:140:GLU:HG3	1.94	0.49
1:A:75:THR:O	1:A:89:GLN:HA	2.12	0.49
1:A:79:ASN:OD1	1:A:81:ASN:HB2	2.11	0.49
1:A:380:PRO:HB3	1:A:385:PHE:CD1	2.48	0.49
1:A:121:LYS:HG3	5:A:851:HOH:O	2.11	0.49
1:A:179:ASN:ND2	1:A:191:ARG:HE	2.10	0.49
1:A:331:LEU:N	1:A:331:LEU:HD23	2.28	0.49
1:C:26:ASN:C	1:C:26:ASN:ND2	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:HIS:CD2	1:C:120:LYS:NZ	2.58	0.49
1:C:223:THR:O	1:C:266:GLY:HA3	2.13	0.49
1:C:330:THR:C	1:C:331:LEU:HD12	2.33	0.49
1:A:172:LEU:HD13	1:A:423:PHE:CD1	2.48	0.49
1:A:322:ILE:HG23	1:A:344:VAL:HG11	1.95	0.49
1:C:40:VAL:CG2	1:C:571:LEU:HD13	2.41	0.48
1:C:331:LEU:HD12	1:C:331:LEU:N	2.28	0.48
1:A:109:ARG:NE	1:A:388:GLN:HE21	2.12	0.48
1:A:381:SER:CB	1:A:407:ILE:HG22	2.43	0.48
2:D:22:LYS:HE3	2:D:24:ALA:O	2.13	0.48
1:A:90:HIS:CD2	1:A:120:LYS:HE2	2.49	0.48
1:A:90:HIS:HD2	1:A:120:LYS:HZ3	1.61	0.48
1:A:295:GLU:OE1	1:A:368:ALA:HB1	2.13	0.48
1:A:429:LEU:N	1:A:429:LEU:CD1	2.77	0.48
1:C:222:LYS:NZ	2:D:8:GLU:OE1	2.46	0.48
1:C:429:LEU:HD12	1:C:429:LEU:N	2.28	0.48
1:A:252:GLY:HA3	1:A:300:GLY:O	2.14	0.47
1:A:494:ASP:CG	1:A:496:LYS:HZ2	2.17	0.47
1:A:172:LEU:HD13	1:A:423:PHE:HA	1.95	0.47
1:C:36:ASN:C	1:C:36:ASN:OD1	2.52	0.47
1:C:259:TRP:CD2	1:C:425:VAL:HG13	2.49	0.47
1:A:335:ASN:C	1:A:335:ASN:ND2	2.65	0.47
1:A:364:ASP:C	1:A:364:ASP:OD1	2.52	0.47
1:A:405:ASN:ND2	5:A:762:HOH:O	2.47	0.47
1:A:491:ASP:OD2	1:A:496:LYS:NZ	2.32	0.47
1:C:230:LYS:NZ	2:D:38:ASN:HD21	2.13	0.47
1:C:268:ASN:HD22	1:C:293:HIS:HA	1.78	0.47
1:A:196:GLY:O	1:A:220:GLY:HA3	2.15	0.47
1:A:442:GLU:H	1:A:442:GLU:CD	2.17	0.47
1:A:555:GLU:HB2	5:A:916:HOH:O	2.15	0.47
1:A:201:VAL:O	1:A:202:ARG:HB2	2.15	0.47
1:A:487:LEU:O	1:A:500:ASN:HA	2.15	0.47
1:C:537:VAL:HG22	1:C:538:PHE:CD2	2.50	0.46
1:A:187:GLU:CB	2:B:55:ILE:HD13	2.27	0.46
1:A:330:THR:C	1:A:331:LEU:HD23	2.35	0.46
1:A:71:PHE:CD2	1:A:99:LYS:HD2	2.50	0.46
1:A:316:THR:HA	1:A:317:PRO:HD3	1.88	0.46
1:A:381:SER:HB3	1:A:407:ILE:HG22	1.97	0.46
1:A:272:MET:HE2	1:A:294:ASP:HB2	1.97	0.46
1:A:419:ARG:NH1	1:A:419:ARG:HG2	2.30	0.46
1:C:303:GLN:NE2	1:C:391:ASP:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:OD1	1:A:299:ALA:HB2	2.16	0.46
1:C:299:ALA:O	1:C:324:ARG:HG3	2.15	0.45
1:A:405:ASN:HB3	1:A:407:ILE:HD12	1.97	0.45
1:A:409:MET:SD	1:A:411:TRP:HE3	2.40	0.45
2:B:6:CYS:HA	2:B:12:CYS:HA	1.98	0.45
1:A:140:GLU:O	2:B:66:PHE:HD2	1.98	0.45
1:A:366:GLU:HG2	1:A:367:PHE:CZ	2.51	0.45
1:C:416:LEU:HB2	1:C:417:PRO:HD2	1.97	0.45
2:D:49:ALA:O	2:D:53:LYS:HG3	2.16	0.45
1:A:331:LEU:HA	1:A:337:ASN:O	2.17	0.45
2:D:23:ILE:CG2	2:D:30:PRO:HD3	2.47	0.45
1:C:491:ASP:OD1	1:C:493:LYS:HB3	2.17	0.45
1:C:531:TRP:N	1:C:532:PRO:HD2	2.32	0.45
1:A:411:TRP:CD1	1:A:411:TRP:C	2.90	0.45
1:C:122:GLN:HB2	1:C:124:ASN:ND2	2.31	0.45
1:C:442:GLU:OE1	1:C:442:GLU:N	2.46	0.45
1:C:27:SER:HA	1:C:28:PRO:HD3	1.86	0.44
1:C:322:ILE:HG23	1:C:344:VAL:HG11	1.99	0.44
2:B:23:ILE:HD12	2:B:23:ILE:HA	1.64	0.44
1:C:55:GLU:OE2	4:C:701:PQQ:O2A	2.35	0.44
1:A:33:ASN:H	1:A:36:ASN:HB2	1.81	0.44
1:A:324:ARG:HG2	1:A:384:GLY:HA3	1.99	0.44
1:A:261:GLU:OE1	2:B:16:LYS:NZ	2.51	0.44
1:A:383:MET:CE	1:A:467:TRP:CH2	3.01	0.44
1:C:250:TYR:HA	1:C:275:TRP:O	2.18	0.44
1:C:335:ASN:HD22	1:C:337:ASN:N	2.00	0.44
2:D:30:PRO:HB2	2:D:32:HIS:CE1	2.52	0.44
1:A:370:ARG:HG3	1:A:373:HIS:HB3	2.00	0.44
1:A:191:ARG:NH1	2:B:44:ILE:CG2	2.81	0.44
1:C:59:LEU:HD22	1:C:111:LEU:HB2	1.99	0.44
1:C:206:ASP:OD1	1:C:206:ASP:N	2.50	0.44
1:C:232:GLY:O	1:C:256:PRO:HA	2.18	0.44
1:C:538:PHE:O	1:C:539:ASP:HB2	2.18	0.44
2:D:16:LYS:HG2	5:D:493:HOH:O	2.17	0.44
1:A:51:LEU:HD22	1:C:51:LEU:HD22	1.99	0.44
1:A:211:ASN:ND2	1:A:337:ASN:OD1	2.38	0.44
2:B:40:GLN:HG3	5:B:70:HOH:O	2.18	0.43
1:A:383:MET:HE2	1:A:467:TRP:CZ3	2.53	0.43
1:C:58:PRO:HG3	1:C:566:LEU:HD13	2.00	0.43
1:A:51:LEU:CD2	1:C:51:LEU:HD22	2.48	0.43
1:A:51:LEU:HB3	1:A:52:ASN:H	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLY:HA3	5:A:728:HOH:O	2.17	0.43
1:A:322:ILE:CG2	1:A:344:VAL:HG11	2.47	0.43
1:C:106:VAL:O	1:C:106:VAL:HG23	2.18	0.43
1:C:542:ASP:O	1:C:545:ALA:HB3	2.18	0.43
1:A:218:GLY:O	1:A:222:LYS:HG3	2.18	0.43
1:A:298:PHE:O	1:A:299:ALA:C	2.56	0.43
1:A:372:ASP:OD2	2:B:28:TYR:OH	2.29	0.43
1:C:320:SER:HA	1:C:329:TYR:O	2.18	0.43
1:A:108:ASP:CG	1:A:121:LYS:HE2	2.39	0.43
1:C:252:GLY:HA3	1:C:300:GLY:O	2.18	0.43
1:C:467:TRP:CZ2	1:C:532:PRO:HD3	2.53	0.43
1:A:223:THR:O	1:A:266:GLY:HA3	2.18	0.43
1:C:536:LEU:C	1:C:536:LEU:HD23	2.39	0.43
1:A:12:GLY:HA3	1:A:515:SER:HB2	2.01	0.43
1:A:237:TRP:CZ2	4:A:701:PQQ:C6A	3.01	0.43
2:B:20:PRO:HB2	2:B:22:LYS:O	2.19	0.42
1:A:374:LYS:HE2	1:A:410:ASP:HB3	2.01	0.42
1:C:474:LYS:HG3	5:C:852:HOH:O	2.18	0.42
1:C:298:PHE:O	1:C:299:ALA:C	2.58	0.42
1:A:320:SER:HA	1:A:329:TYR:O	2.19	0.42
1:C:179:ASN:HD21	1:C:191:ARG:HE	1.63	0.42
1:A:371:MET:CE	1:A:415:MET:HG2	2.49	0.42
1:C:114:GLY:O	1:C:117:GLN:HB2	2.19	0.42
1:C:231:ILE:HD13	2:D:37:LEU:CD1	2.49	0.42
2:B:29:ASP:HA	2:B:30:PRO:HD2	1.81	0.42
1:C:191:ARG:HH11	1:C:191:ARG:HD2	1.63	0.42
1:A:383:MET:HG2	1:A:531:TRP:CE3	2.54	0.42
1:A:37:VAL:HG11	1:A:498:LEU:HB3	2.02	0.42
1:A:271:THR:O	1:A:273:THR:HG22	2.19	0.42
1:A:360:THR:HA	1:A:361:PRO:HD3	1.92	0.42
1:A:510:SER:HA	1:A:511:PRO:HD3	1.86	0.42
1:A:388:GLN:NE2	5:A:764:HOH:O	2.43	0.41
1:C:12:GLY:HA3	1:C:515:SER:HB2	2.01	0.41
1:C:542:ASP:HB3	1:C:545:ALA:HB2	2.00	0.41
1:A:198:ASP:OD2	1:A:217:PHE:HB3	2.20	0.41
1:A:319:LEU:C	1:A:319:LEU:CD2	2.84	0.41
1:C:345:ASP:CG	1:C:346:PRO:HD2	2.40	0.41
1:A:531:TRP:CE3	4:A:701:PQQ:O4	2.73	0.41
1:C:316:THR:HA	1:C:317:PRO:HD3	1.76	0.41
1:A:142:GLU:CD	2:B:50:ARG:NH1	2.74	0.41
1:C:187:GLU:OE2	2:D:55:ILE:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HD12	1:A:424:PHE:CE2	2.55	0.41
2:B:49:ALA:O	2:B:53:LYS:HB2	2.21	0.41
1:A:271:THR:O	1:A:273:THR:HG23	2.20	0.41
1:C:463:LYS:NZ	1:C:559:HIS:CE1	2.89	0.41
1:A:201:VAL:HG12	1:A:203:LEU:HD21	2.02	0.41
1:A:345:ASP:CG	1:A:346:PRO:HD2	2.40	0.41
1:A:390:VAL:O	1:A:469:GLY:HA3	2.20	0.41
2:B:51:ASN:HD21	2:B:54:ARG:HH21	1.65	0.41
2:B:51:ASN:O	2:B:55:ILE:HG23	2.20	0.41
5:C:914:HOH:O	2:D:9:PRO:HA	2.19	0.41
1:A:18:THR:HB	1:A:23:SER:HB3	2.03	0.41
1:A:37:VAL:CG1	1:A:498:LEU:HB3	2.51	0.41
1:A:121:LYS:HG3	1:A:121:LYS:H	1.81	0.41
1:A:167:CYS:O	1:A:235:THR:HB	2.20	0.41
1:C:128:LEU:N	1:C:128:LEU:CD2	2.82	0.41
1:C:463:LYS:CE	1:C:559:HIS:CE1	3.04	0.41
1:C:535:GLY:HA2	1:C:540:LEU:HB2	2.03	0.41
1:A:130:LEU:CD2	1:A:137:ILE:HG12	2.51	0.41
1:A:179:ASN:HD22	1:A:191:ARG:HE	1.67	0.41
1:A:277:ARG:HD3	1:A:277:ARG:HH11	1.68	0.40
1:C:124:ASN:ND2	1:C:124:ASN:C	2.74	0.40
1:C:304:MET:CE	1:C:321:HIS:CD2	3.04	0.40
1:A:267:ASP:OD1	2:B:13:TRP:HB2	2.20	0.40
1:A:311:VAL:O	1:A:312:ASN:HB2	2.20	0.40
1:C:335:ASN:ND2	1:C:337:ASN:HB2	2.37	0.40
1:A:243:ASP:O	1:A:247:ASN:N	2.52	0.40
2:B:34:PRO:O	2:B:37:LEU:HB2	2.21	0.40
1:C:335:ASN:ND2	1:C:337:ASN:CB	2.85	0.40
1:C:472:TYR:CD2	1:C:472:TYR:C	2.95	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	569/571 (100%)	527 (93%)	40 (7%)	2 (0%)	34	48
1	C	569/571 (100%)	533 (94%)	35 (6%)	1 (0%)	47	62
2	B	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
2	D	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
All	All	1272/1280 (99%)	1187 (93%)	82 (6%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	A	420	ALA
1	C	388	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/452 (100%)	406 (90%)	46 (10%)	7	10
1	C	452/452 (100%)	419 (93%)	33 (7%)	14	22
2	B	58/58 (100%)	53 (91%)	5 (9%)	10	16
2	D	58/58 (100%)	50 (86%)	8 (14%)	3	4
All	All	1020/1020 (100%)	928 (91%)	92 (9%)	9	14

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	51	LEU
1	A	80	LEU
1	A	85	LYS
1	A	97	SER
1	A	120	LYS
1	A	121	LYS
1	A	128	LEU

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Mol	Chain	Res	Type
1	A	133	LYS
1	A	163	VAL
1	A	165	MET
1	A	171	GLU
1	A	172	LEU
1	A	178	VAL
1	A	183	LEU
1	A	184	LYS
1	A	199	ASP
1	A	246	LEU
1	A	273	THR
1	A	314	LYS
1	A	316	THR
1	A	331	LEU
1	A	335	ASN
1	A	338	LEU
1	A	350	VAL
1	A	353	LYS
1	A	354	VAL
1	A	358	THR
1	A	360	THR
1	A	388	GLN
1	A	398	ARG
1	A	405	ASN
1	A	416	LEU
1	A	429	LEU
1	A	440	LYS
1	A	445	GLN
1	A	455	LYS
1	A	477	LEU
1	A	478	VAL
1	A	493	LYS
1	A	498	LEU
1	A	515	SER
1	A	519	LYS
1	A	540	LEU
1	A	556	LEU
1	A	571	LEU
2	B	8	GLU
2	B	23	ILE
2	B	55	ILE
2	B	59	LYS

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Mol	Chain	Res	Type
2	B	65	VAL
1	C	18	THR
1	C	26	ASN
1	C	29	LEU
1	C	51	LEU
1	C	59	LEU
1	C	121	LYS
1	C	124	ASN
1	C	128	LEU
1	C	133	LYS
1	C	161	ASP
1	C	162	THR
1	C	163	VAL
1	C	164	LEU
1	C	221	THR
1	C	222	LYS
1	C	246	LEU
1	C	335	ASN
1	C	342	GLU
1	C	353	LYS
1	C	388	GLN
1	C	411	TRP
1	C	416	LEU
1	C	429	LEU
1	C	455	LYS
1	C	477	LEU
1	C	478	VAL
1	C	487	LEU
1	C	537	VAL
1	C	539	ASP
1	C	540	LEU
1	C	554	ARG
1	C	556	LEU
1	C	571	LEU
2	D	22	LYS
2	D	23	ILE
2	D	37	LEU
2	D	55	ILE
2	D	57	ASN
2	D	61	SER
2	D	65	VAL
2	D	67	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	90	HIS
1	A	117	GLN
1	A	179	ASN
1	A	216	GLN
1	A	268	ASN
1	A	303	GLN
1	A	335	ASN
1	A	388	GLN
1	A	405	ASN
1	A	436	ASN
1	A	558	ASN
1	A	559	HIS
2	B	51	ASN
1	C	26	ASN
1	C	81	ASN
1	C	90	HIS
1	C	94	GLN
1	C	124	ASN
1	C	179	ASN
1	C	268	ASN
1	C	289	GLN
1	C	302	ASN
1	C	303	GLN
1	C	309	GLN
1	C	321	HIS
1	C	335	ASN
1	C	388	GLN
1	C	405	ASN
1	C	422	GLN
1	C	558	ASN
1	C	559	HIS
2	D	4	GLN
2	D	38	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 monosaccharides 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	$\#\|Z\| > 2$
4	PQQ	C	701	3	23,26,26	3.97	10 (43%)	29,40,40	2.69	11 (37%)
4	PQQ	A	701	3	23,26,26	4.02	12 (52%)	29,40,40	2.37	11 (37%)

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	C	701	3	-	4/10/28/28	0/3/3/3
4	PQQ	A	701	3	-	3/10/28/28	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	PQQ	C2-C2X	-8.65	1.38	1.50
4	C	701	PQQ	O4-C4	7.83	1.39	1.23
4	C	701	PQQ	O5-C5	7.54	1.39	1.23
4	C	701	PQQ	C6A-C5	-7.53	1.40	1.50
4	A	701	PQQ	O4-C4	7.47	1.39	1.23
4	A	701	PQQ	C7-C7X	-6.74	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	PQQ	C2-C2X	-6.64	1.41	1.50
4	A	701	PQQ	C6A-C5	-6.58	1.42	1.50
4	C	701	PQQ	C9-C9X	-6.47	1.39	1.50
4	A	701	PQQ	O5-C5	6.27	1.36	1.23
4	C	701	PQQ	C7-C7X	-6.18	1.42	1.50
4	A	701	PQQ	C3A-C4	-4.85	1.39	1.48
4	A	701	PQQ	C5-C4	-4.79	1.37	1.53
4	A	701	PQQ	C9-C9X	-4.79	1.42	1.50
4	C	701	PQQ	C5-C4	-4.55	1.38	1.53
4	A	701	PQQ	C6A-N6	3.79	1.35	1.32
4	C	701	PQQ	C3A-C4	-3.31	1.42	1.48
4	A	701	PQQ	O2B-C2X	-2.77	1.22	1.30
4	C	701	PQQ	O9B-C9X	-2.72	1.22	1.30
4	A	701	PQQ	O9B-C9X	-2.64	1.22	1.30
4	C	701	PQQ	C3-C3A	-2.44	1.35	1.40
4	A	701	PQQ	C3-C3A	-2.00	1.36	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	701	PQQ	C9-C9A-C1A	7.11	128.71	122.88
4	C	701	PQQ	C9-C9A-C6A	-6.26	113.31	121.68
4	A	701	PQQ	C9-C9A-C1A	5.30	127.23	122.88
4	A	701	PQQ	C9-C9A-C6A	-5.28	114.62	121.68
4	C	701	PQQ	O9B-C9X-C9	4.56	127.31	114.39
4	A	701	PQQ	O9B-C9X-O9A	-3.99	114.50	123.35
4	C	701	PQQ	O7B-C7X-O7A	-3.98	114.52	123.35
4	C	701	PQQ	O5-C5-C6A	-3.70	117.92	121.84
4	C	701	PQQ	C8-C7-C7X	3.70	127.55	119.57
4	A	701	PQQ	O9B-C9X-C9	3.65	124.73	114.39
4	C	701	PQQ	O7B-C7X-C7	3.54	122.74	114.69
4	C	701	PQQ	C7X-C7-N6	-3.51	111.30	116.48
4	A	701	PQQ	C7X-C7-N6	-3.47	111.36	116.48
4	A	701	PQQ	C8-C7-C7X	3.13	126.33	119.57
4	C	701	PQQ	O9B-C9X-O9A	-2.85	117.02	123.35
4	A	701	PQQ	O2B-C2X-C2	2.83	121.14	114.69
4	A	701	PQQ	O7B-C7X-C7	2.61	120.62	114.69
4	A	701	PQQ	C3A-C4-C5	2.60	119.65	118.14
4	C	701	PQQ	O9A-C9X-C9	-2.49	115.59	122.23
4	A	701	PQQ	O2B-C2X-O2A	-2.12	118.63	123.35
4	C	701	PQQ	C9A-C9-C9X	-2.12	120.95	123.95
4	A	701	PQQ	C6A-N6-C7	-2.03	114.50	117.91

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	PQQ	C8-C9-C9X-O9B
4	C	701	PQQ	C8-C9-C9X-O9A
4	A	701	PQQ	C9A-C9-C9X-O9B
4	C	701	PQQ	C9A-C9-C9X-O9A
4	C	701	PQQ	C9A-C9-C9X-O9B
4	C	701	PQQ	C8-C9-C9X-O9B
4	A	701	PQQ	C8-C9-C9X-O9A

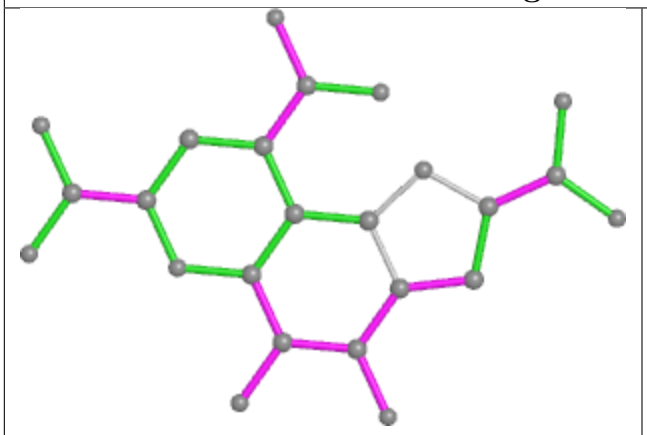
There are no ring outliers.

2 monomers are involved in 6 short contacts:

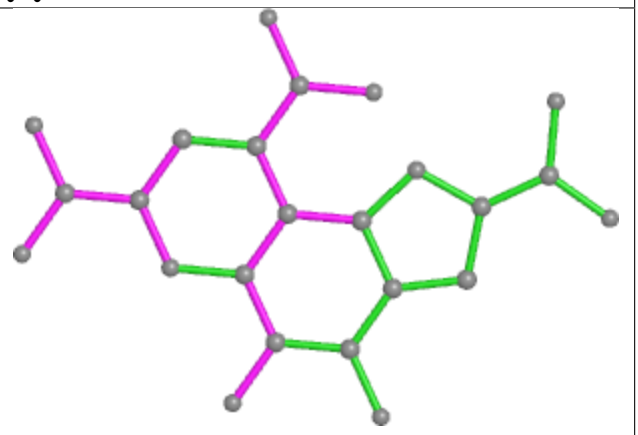
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	701	PQQ	3	0
4	A	701	PQQ	3	0

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 then 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.

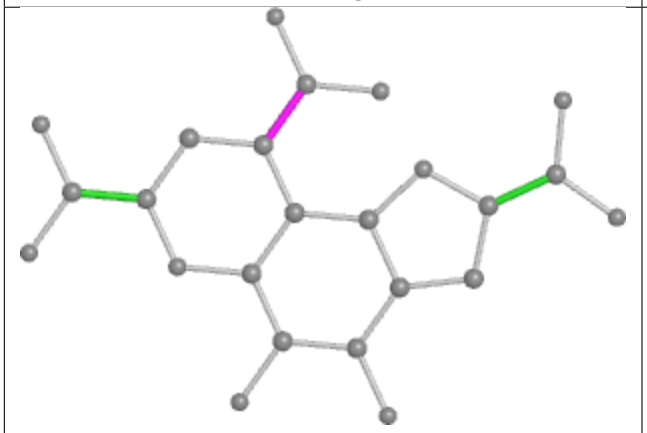
Ligand PQQ C 701



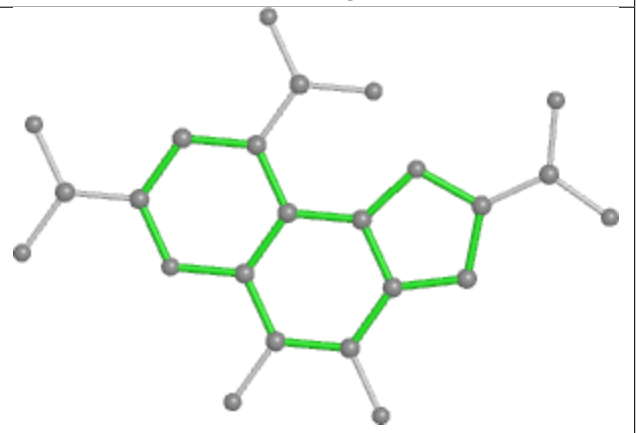
Bond lengths



Bond angles

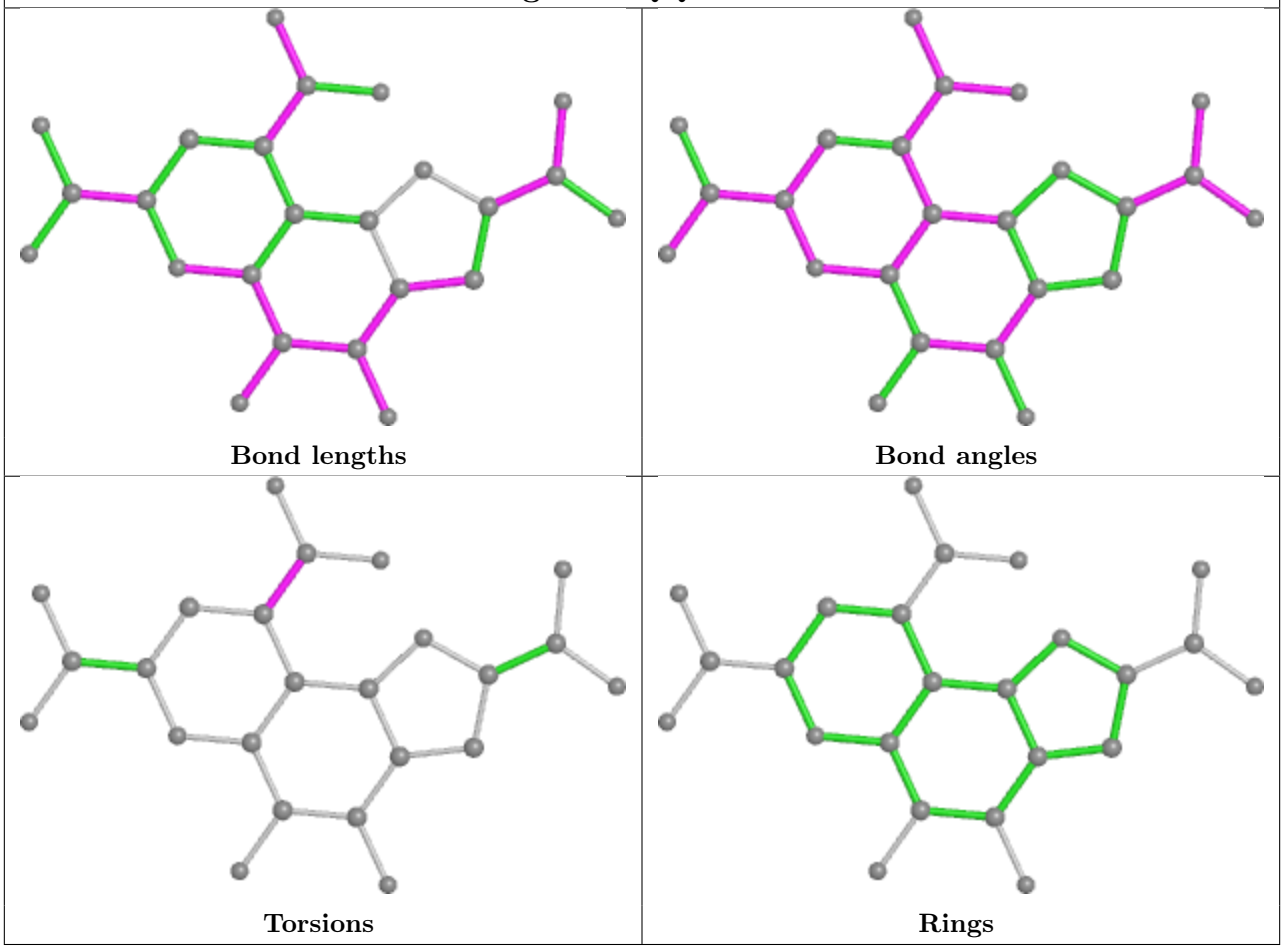


Torsions



Rings

Ligand PQQ A 701



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	571/571 (100%)	-0.88	0	100	100	2, 12, 23, 34	0
1	C	571/571 (100%)	-0.74	0	100	100	2, 6, 17, 26	0
2	B	69/69 (100%)	-0.21	3 (4%)	35	33	18, 27, 50, 66	0
2	D	69/69 (100%)	-0.21	4 (5%)	23	22	5, 17, 47, 60	0
All	All	1280/1280 (100%)	-0.75	7 (0%)	91	89	2, 10, 27, 66	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	68	VAL	3.9
2	D	68	VAL	3.4
2	B	67	ASP	3.4
2	D	69	LYS	2.8
2	D	60	SER	2.4
2	D	63	ASN	2.3
2	B	69	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

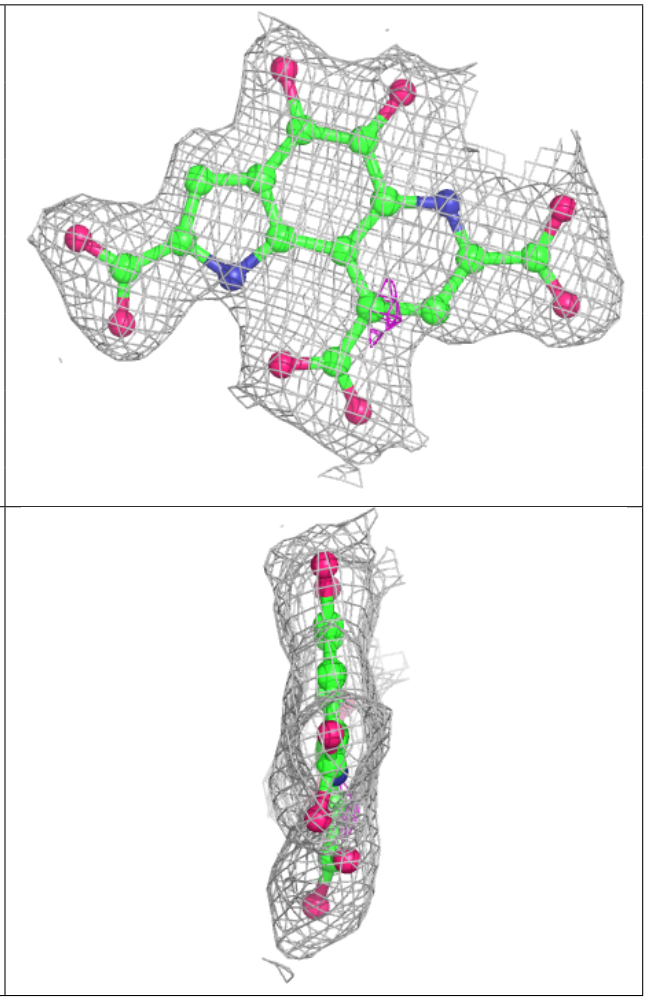
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	C	702	1/1	0.95	0.06	19,19,19,19	0
4	PQQ	A	701	24/24	0.96	0.10	8,11,11,12	0
4	PQQ	C	701	24/24	0.96	0.10	2,2,3,3	0
3	CA	A	702	1/1	0.99	0.05	21,21,21,21	0

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.

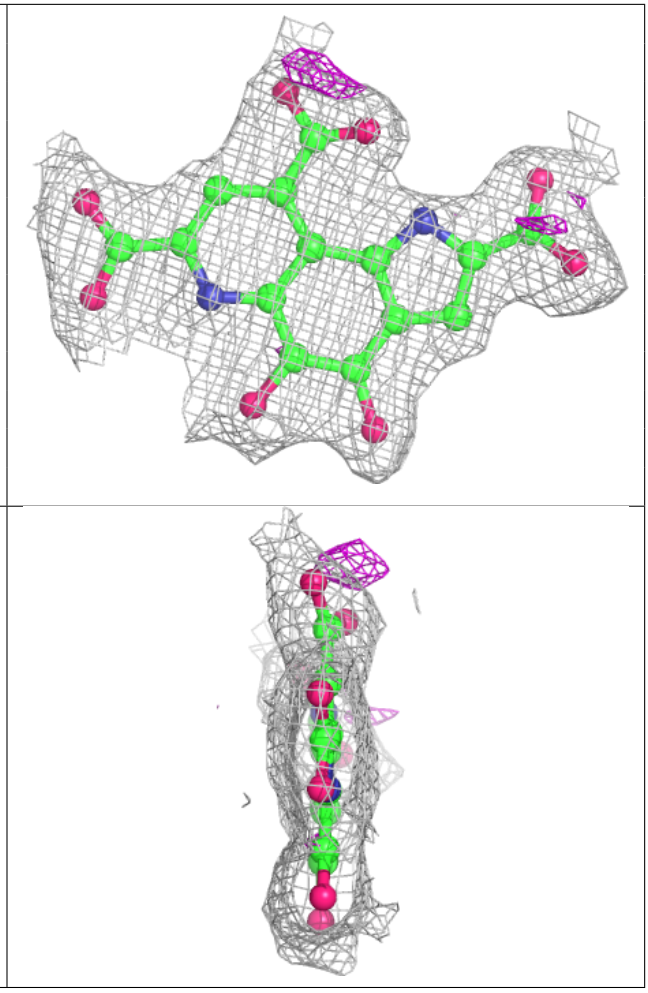
Electron density around PQQ A 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PQQ C 701:

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.