



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:17 AM GMT

PDB ID : 3OMA
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with K362M mutation
Authors : Liu, J.; Qin, L.; Ferguson-Miller, S.
Deposited on : 2010-08-26
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

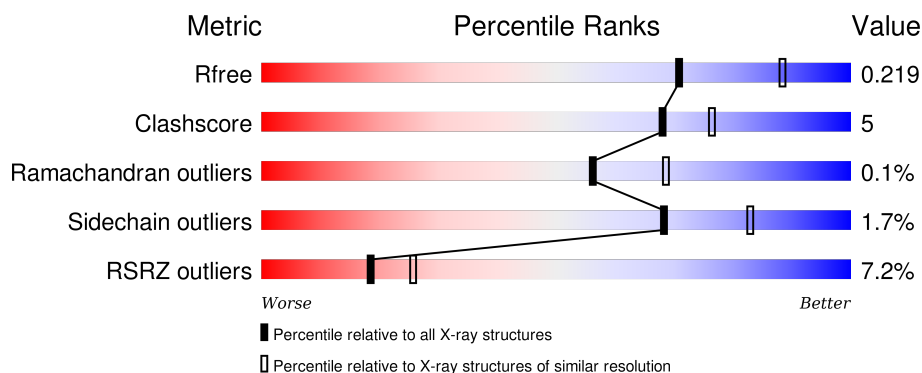
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	535	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
1	C	535	<div> <div>11%</div> <div>86%</div> <div>13%</div> </div>
2	B	256	<div> <div>3%</div> <div>95%</div> <div></div> </div>
2	D	256	<div> <div>7%</div> <div>92%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HTH	B	286	-	-	-	X
4	DMU	A	1005	-	-	-	X
4	DMU	A	7	-	-	-	X
4	DMU	B	2	-	-	-	X
4	DMU	B	3	-	-	-	X
4	DMU	C	10	-	-	-	X
4	DMU	C	9	-	-	-	X
5	TRD	A	1009	-	-	-	X
5	TRD	B	4	-	-	-	X
5	TRD	D	3	-	-	-	X
6	HEA	A	1	X	-	-	-
6	HEA	A	2	X	-	-	-
6	HEA	C	1	X	-	-	-
6	HEA	C	2	X	-	-	-
8	MG	A	6	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13395 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 Cytochrome c oxidase, aa3 type, subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4159	2784	654	689	32			
1	C	531	Total	C	N	O	S	0	0	0
			4121	2761	646	683	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	MET	LYS	ENGINEERED MUTATION	UNP Q3J5A7
C	362	MET	LYS	ENGINEERED MUTATION	UNP Q3J5A7

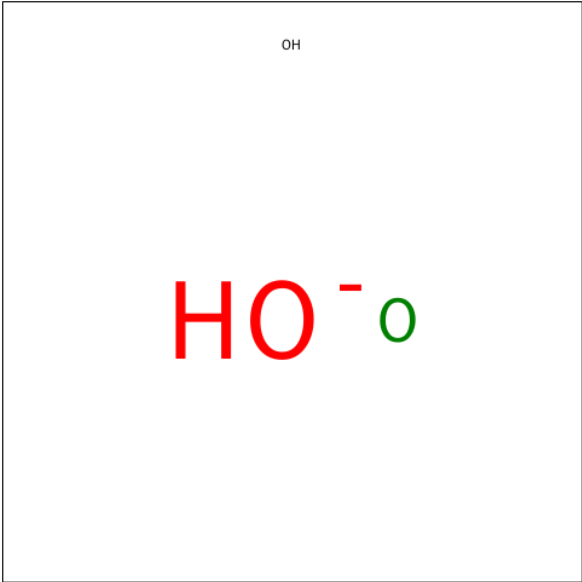
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2018	1316	333	363	6			
2	D	256	Total	C	N	O	S	0	0	0
			1999	1305	326	362	6			

There are 8 discrepancies between the modelled and reference sequences:

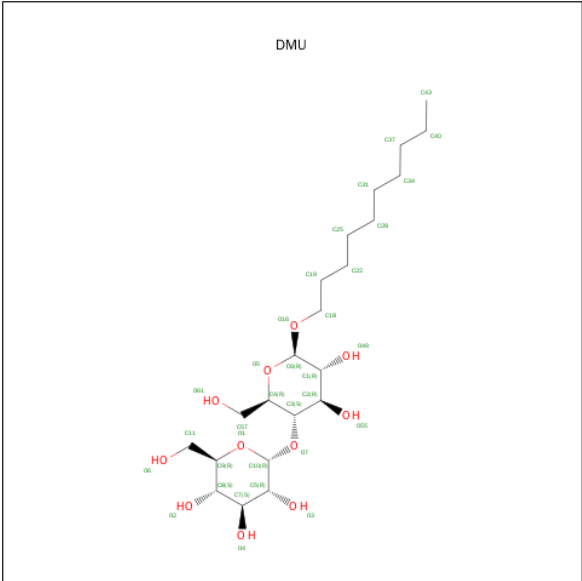
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	284	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	285	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	284	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	285	HIS	-	EXPRESSION TAG	UNP Q3J5G0

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 4 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



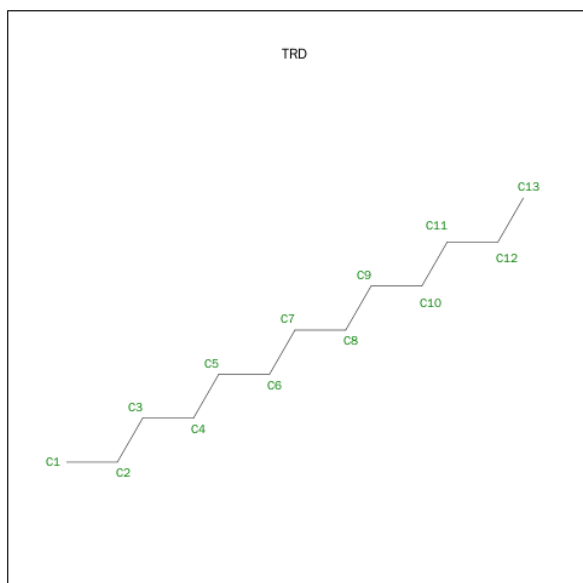
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			22	16 6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	16	6		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			33	22	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



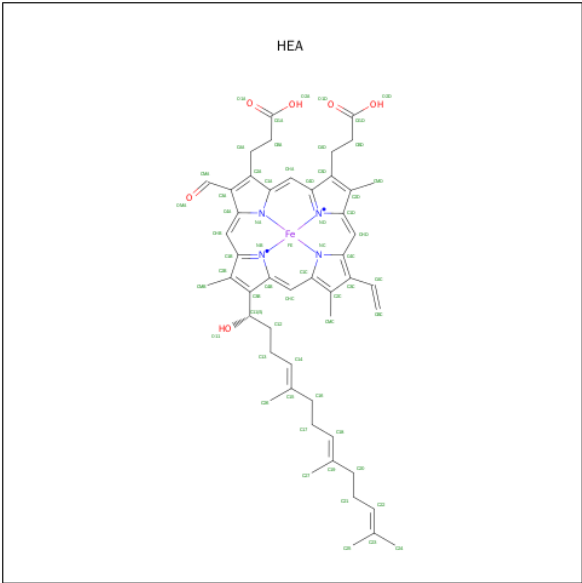
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 7 7	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	B	1	Total C 9 9	0	0
5	C	1	Total C 13 13	0	0
5	D	1	Total C 13 13	0	0
5	D	1	Total C 7 7	0	0

- Molecule 6 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Fe N O 60 49 1 4 6	0	0
6	A	1	Total C Fe N O 60 49 1 4 6	0	0
6	C	1	Total C Fe N O 60 49 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cu	0	0
			1	1		
7	A	1	Total	Cu	0	0
			1	1		
7	D	1	Total	Cu	0	0
			1	1		
7	C	1	Total	Cu	0	0
			1	1		

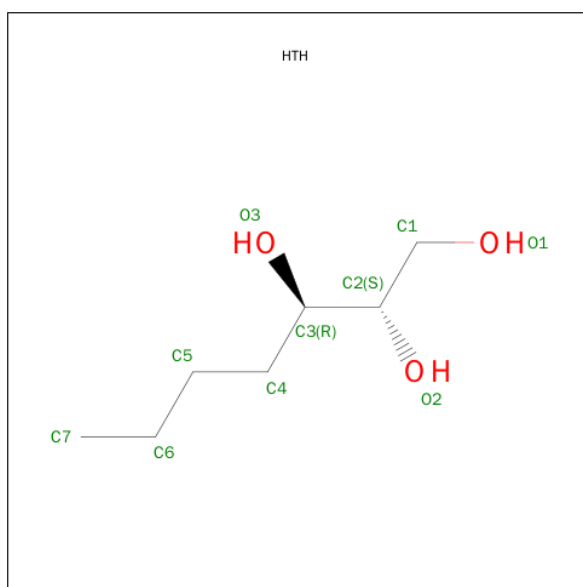
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is (2S,3R)-HEPTANE-1,2,3-TRIOL (three-letter code: HTH) (formula: C₇H₁₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Cu	0	0
			1	1		
11	D	1	Total	Cu	0	0
			1	1		

- Molecule 12 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	2	Total	Cd	0	0
			2	2		
12	D	2	Total	Cd	0	0
			2	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	132	Total	O	0	0
			132	132		
13	B	134	Total	O	0	0
			134	134		

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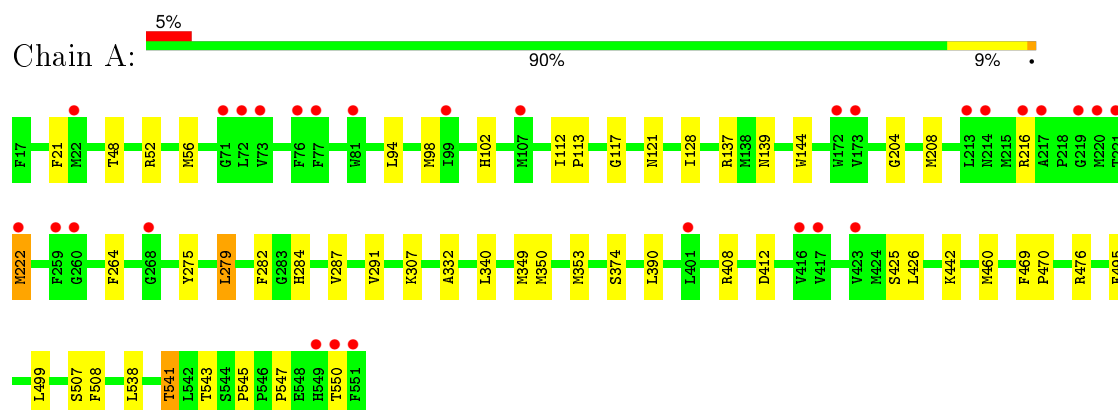
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	82	Total 82	O 82	0	0
13	D	104	Total 104	O 104	0	0

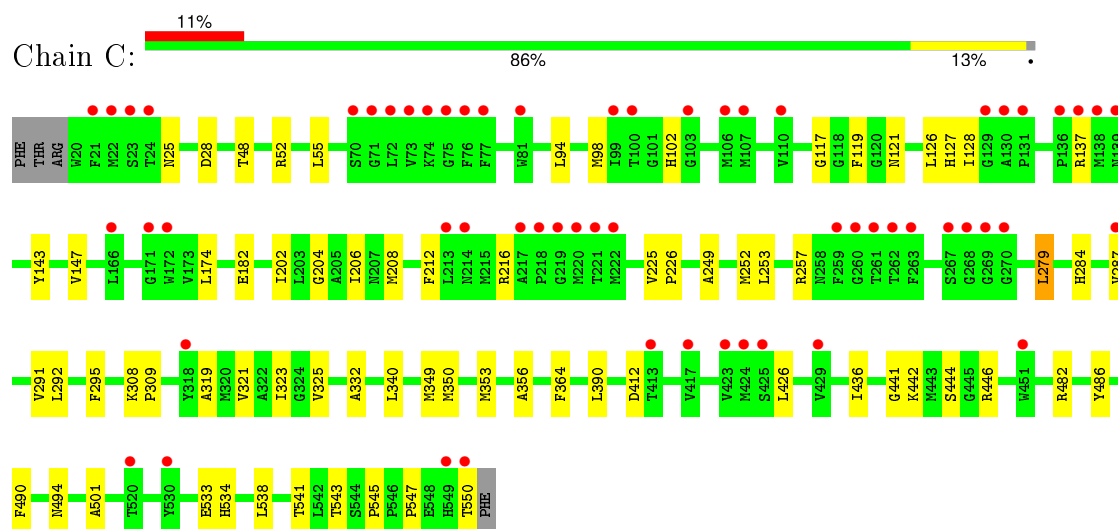
3 Residue-property plots [i](#)

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.

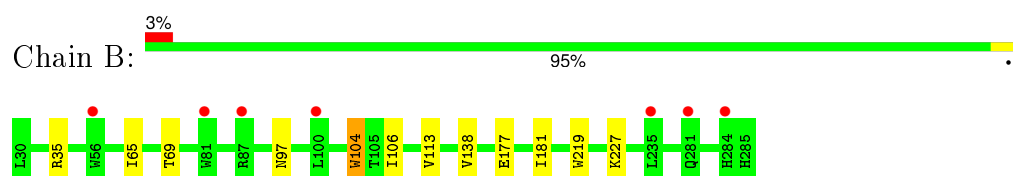
- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I



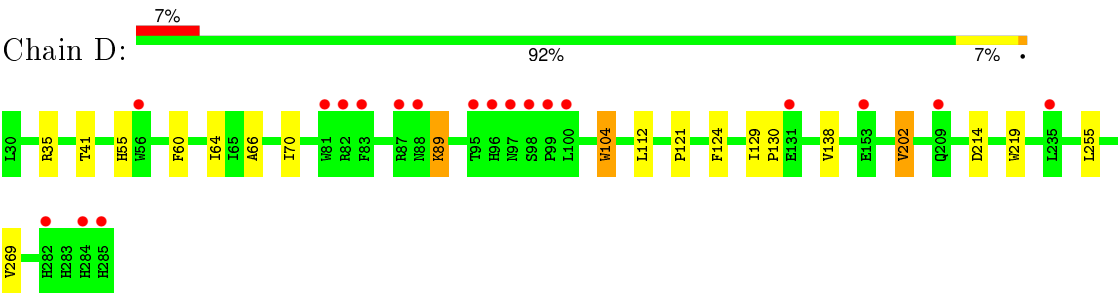
- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I



- Molecule 2: Cytochrome c oxidase subunit 2



● Molecule 2: Cytochrome c oxidase subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.02Å 131.58Å 176.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.30) 97.6 (49.37-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.219 0.192 , 0.219	Depositor DCC
R_{free} test set	3771 reflections (3.08%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.6	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 126383 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13395	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, CU1, OH, CA, TRD, CD, DMU, HTH, CU, HEA

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	0.60	0/4311	0.56	0/5888
1	C	0.53	0/4272	0.54	0/5837
2	B	0.62	0/2080	0.57	0/2848
2	D	0.52	0/2060	0.54	0/2824
All	All	0.57	0/12723	0.55	0/17397

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4159	0	4051	43	0
1	C	4121	0	4015	48	0
2	B	2018	0	1969	7	0
2	D	1999	0	1936	17	0
3	A	1	0	0	1	0
3	C	1	0	0	1	0
4	A	44	0	62	1	0
4	B	122	0	147	0	0
4	C	79	0	84	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	46	0	42	3	0
5	A	47	0	92	1	0
5	B	9	0	17	1	0
5	C	13	0	28	0	0
5	D	20	0	41	1	0
6	A	120	0	108	6	0
6	C	120	0	108	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	10	0	16	1	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	A	132	0	0	4	0
13	B	134	0	0	1	0
13	C	82	0	0	4	0
13	D	104	0	0	1	0
All	All	13395	0	12716	120	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 5.

The worst 5 of 120 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)
2:D:89:LYS:NZ	2:D:89:LYS:HB3	1.43	1.06
2:D:89:LYS:HB3	2:D:89:LYS:HZ2	0.85	0.99
1:C:534:HIS:HD2	13:C:623:HOH:O	1.44	0.98
2:D:89:LYS:NZ	2:D:89:LYS:CB	2.30	0.89
2:D:89:LYS:CB	2:D:89:LYS:HZ2	1.81	0.86

There are no symmetry-related clashes.

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	533/535 (100%)	520 (98%)	13 (2%)	0	100	100
1	C	529/535 (99%)	516 (98%)	13 (2%)	0	100	100
2	B	254/256 (99%)	248 (98%)	5 (2%)	1 (0%)	39	48
2	D	254/256 (99%)	245 (96%)	9 (4%)	0	100	100
All	All	1570/1582 (99%)	1529 (97%)	40 (2%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	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	424/435 (98%)	416 (98%)	8 (2%)	65	81
1	C	420/435 (97%)	415 (99%)	5 (1%)	78	89
2	B	213/215 (99%)	210 (99%)	3 (1%)	74	86
2	D	209/215 (97%)	204 (98%)	5 (2%)	57	74
All	All	1266/1300 (97%)	1245 (98%)	21 (2%)	68	83

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	104	TRP
1	C	137	ARG
2	D	89	LYS
2	B	35	ARG
2	D	104	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 41 ligands modelled in this entry, 2 are modelled with single atom and 14 are monoatomic - leaving 25 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	$\# Z > 2$
6	HEA	A	1	1	40,67,67	1.39	3 (7%)	41,103,103	1.83	8 (19%)
4	DMU	A	1005	-	22,22,34	0.55	0	27,27,45	0.90	1 (3%)
5	TRD	A	1009	-	6,6,12	0.30	0	5,5,11	0.35	0
5	TRD	A	1013	-	6,6,12	0.31	0	5,5,11	0.37	0
5	TRD	A	1015	-	6,6,12	0.31	0	5,5,11	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEA	A	2	1,13	40,67,67	1.33	5 (12%)	41,103,103	1.60	7 (17%)
5	TRD	A	3	-	12,12,12	0.35	0	11,11,11	0.35	0
5	TRD	A	552	-	12,12,12	0.27	0	11,11,11	0.48	0
4	DMU	A	7	-	22,22,34	0.54	0	27,27,45	0.86	1 (3%)
4	DMU	B	1	-	34,34,34	0.57	0	45,45,45	1.18	2 (4%)
4	DMU	B	2	-	34,34,34	0.54	0	45,45,45	0.98	3 (6%)
10	HTH	B	286	-	9,9,9	0.32	0	8,10,10	0.75	0
4	DMU	B	3	-	34,34,34	0.55	0	45,45,45	0.61	0
5	TRD	B	4	-	8,8,12	0.26	0	7,7,11	0.45	0
4	DMU	B	6	-	24,24,34	0.53	0	35,35,45	0.75	0
6	HEA	C	1	1	40,67,67	1.38	3 (7%)	41,103,103	1.59	8 (19%)
4	DMU	C	10	-	34,34,34	0.63	0	45,45,45	0.86	1 (2%)
6	HEA	C	2	1,13	40,67,67	1.40	3 (7%)	41,103,103	1.60	9 (21%)
4	DMU	C	5	-	24,24,34	0.52	0	35,35,45	0.65	0
5	TRD	C	552	-	12,12,12	0.26	0	11,11,11	0.52	0
4	DMU	C	9	-	24,24,34	0.59	0	35,35,45	0.93	1 (2%)
5	TRD	D	14	-	6,6,12	0.26	0	5,5,11	0.37	0
5	TRD	D	3	-	12,12,12	0.21	0	11,11,11	0.58	0
4	DMU	D	4	-	24,24,34	0.54	0	35,35,45	0.65	0
4	DMU	D	8	-	24,24,34	0.53	0	35,35,45	0.67	0

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
6	HEA	A	1	1	2/2/7/16	0/24/76/76	0/0/8/8
4	DMU	A	1005	-	-	0/13/33/59	0/1/1/2
5	TRD	A	1009	-	-	0/4/4/10	0/0/0/0
5	TRD	A	1013	-	-	0/4/4/10	0/0/0/0
5	TRD	A	1015	-	-	0/4/4/10	0/0/0/0
6	HEA	A	2	1,13	3/3/7/16	0/24/76/76	0/0/8/8
5	TRD	A	3	-	-	0/10/10/10	0/0/0/0
5	TRD	A	552	-	-	0/10/10/10	0/0/0/0
4	DMU	A	7	-	-	0/13/33/59	0/1/1/2
4	DMU	B	1	-	-	0/19/59/59	0/2/2/2
4	DMU	B	2	-	-	0/19/59/59	0/2/2/2
10	HTH	B	286	-	-	0/10/10/10	0/0/0/0
4	DMU	B	3	-	-	0/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRD	B	4	-	-	0/6/6/10	0/0/0/0
4	DMU	B	6	-	-	0/8/48/59	0/2/2/2
6	HEA	C	1	1	2/2/7/16	0/24/76/76	0/0/8/8
4	DMU	C	10	-	-	0/19/59/59	0/2/2/2
6	HEA	C	2	1,13	3/3/7/16	0/24/76/76	0/0/8/8
4	DMU	C	5	-	-	0/8/48/59	0/2/2/2
5	TRD	C	552	-	-	0/10/10/10	0/0/0/0
4	DMU	C	9	-	-	0/8/48/59	0/2/2/2
5	TRD	D	14	-	-	0/4/4/10	0/0/0/0
5	TRD	D	3	-	-	0/10/10/10	0/0/0/0
4	DMU	D	4	-	-	0/8/48/59	0/2/2/2
4	DMU	D	8	-	-	0/8/48/59	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	HEA	C3A-C2A	-4.84	1.33	1.40
6	C	1	HEA	C3A-C2A	-4.62	1.34	1.40
6	C	2	HEA	C3A-C2A	-4.25	1.34	1.40
6	C	2	HEA	C3C-C2C	-4.15	1.34	1.40
6	A	2	HEA	C3A-C2A	-3.82	1.35	1.40

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1	HEA	C4B-C3B-C11	-5.11	121.46	127.01
6	C	2	HEA	CAD-CBD-CGD	-3.65	106.05	112.75
6	A	2	HEA	CAD-CBD-CGD	-3.44	106.45	112.75
6	A	1	HEA	CMC-C2C-C1C	-3.33	122.85	128.36
6	C	2	HEA	CAD-C3D-C4D	-3.31	123.41	127.01

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	2	HEA	NB
6	C	2	HEA	NA
6	C	2	HEA	ND
6	C	1	HEA	ND
6	C	1	HEA	NB

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1	HEA	3	0
4	A	1005	DMU	1	0
6	A	2	HEA	3	0
5	A	3	TRD	1	0
10	B	286	HTH	1	0
5	B	4	TRD	1	0
6	C	1	HEA	2	0
6	C	2	HEA	3	0
4	C	9	DMU	1	0
5	D	3	TRD	1	0
4	D	4	DMU	3	0

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	535/535 (100%)	0.16	29 (5%) 29 38	25, 38, 60, 78	0
1	C	531/535 (99%)	0.55	59 (11%) 7 11	32, 54, 78, 92	0
2	B	256/256 (100%)	-0.05	7 (2%) 58 67	25, 42, 60, 66	0
2	D	256/256 (100%)	0.08	19 (7%) 17 25	32, 47, 68, 77	0
All	All	1578/1582 (99%)	0.25	114 (7%) 18 26	25, 45, 70, 92	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	PRO	6.2
1	C	222	MET	6.2
1	C	217	ALA	5.8
1	C	549	HIS	5.7
1	C	77	PHE	5.2

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 carbohydrates 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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	DMU	B	2	33/33	0.77	0.29	9.86	67,69,78,79	25
5	TRD	A	1009	7/13	0.74	0.30	8.10	64,66,67,67	0
4	DMU	A	1005	22/33	0.87	0.20	7.18	45,50,56,57	22
4	DMU	C	9	23/33	0.52	0.29	5.29	96,98,102,102	23
10	HTH	B	286	10/10	0.76	0.41	5.05	71,76,77,77	0
4	DMU	C	10	33/33	0.83	0.23	4.29	81,83,85,85	0
5	TRD	B	4	9/13	0.73	0.30	4.20	70,71,75,75	0
4	DMU	A	7	22/33	0.78	0.20	3.43	46,66,74,76	0
5	TRD	D	3	13/13	0.91	0.27	2.93	54,55,59,59	0
8	MG	A	6	1/1	0.98	0.24	2.55	20,20,20,20	0
4	DMU	B	3	33/33	0.89	0.26	2.54	83,88,92,93	0
5	TRD	A	1013	7/13	0.79	0.23	1.78	56,56,57,57	0
5	TRD	A	3	13/13	0.92	0.20	1.65	42,44,53,54	0
8	MG	C	6	1/1	0.99	0.19	0.88	20,20,20,20	0
6	HEA	A	2	60/60	0.96	0.21	0.65	28,33,46,48	0
4	DMU	B	1	33/33	0.96	0.11	0.60	30,41,58,60	0
6	HEA	C	1	60/60	0.97	0.23	0.58	31,35,51,53	0
11	CU1	B	288	1/1	1.00	0.14	0.37	27,27,27,27	0
6	HEA	A	1	60/60	0.99	0.19	0.27	23,26,34,35	0
11	CU1	D	287	1/1	1.00	0.11	0.02	35,35,35,35	0
7	CU	D	286	1/1	1.00	0.11	-0.16	35,35,35,35	0
5	TRD	D	14	7/13	0.89	0.12	-0.22	56,56,59,59	0
9	CA	A	553	1/1	0.99	0.11	-0.33	30,30,30,30	0
6	HEA	C	2	60/60	0.97	0.16	-0.36	31,38,48,50	0
3	OH	A	706	1/1	0.99	0.14	-1.15	36,36,36,36	0
7	CU	B	287	1/1	1.00	0.11	-1.18	28,28,28,28	0
12	CD	D	9	1/1	0.91	0.04	-2.39	64,64,64,64	1
12	CD	D	288	1/1	0.99	0.06	-2.55	43,43,43,43	0
9	CA	C	7	1/1	0.98	0.05	-3.30	45,45,45,45	0
12	CD	B	9	1/1	0.99	0.05	-4.31	53,53,53,53	1
12	CD	B	8	1/1	0.99	0.07	-6.64	44,44,44,44	0
5	TRD	A	552	13/13	0.85	0.25	-	72,72,75,75	0
5	TRD	A	1015	7/13	0.71	0.35	-	70,70,70,70	0
3	OH	C	706	1/1	0.98	0.22	-	48,48,48,48	0
7	CU	A	5	1/1	0.99	0.15	-	35,35,35,35	0
4	DMU	C	5	23/33	0.85	0.22	-	95,95,96,96	23
4	DMU	D	4	23/33	0.88	0.21	-	81,82,83,83	23
4	DMU	B	6	23/33	0.82	0.19	-	76,77,77,77	23
4	DMU	D	8	23/33	0.78	0.33	-	92,93,97,97	23
7	CU	C	553	1/1	1.00	0.13	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	TRD	C	552	13/13	0.81	0.33	-	83,84,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.