



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2017 – 06:31 PM EDT

PDB ID : 3OMN  
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with D132A mutation in the reduced state  
Authors : Liu, J.; Qin, L.; Ferguson-Miller, S.  
Deposited on : unknown  
Resolution : 2.15 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](mailto: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.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

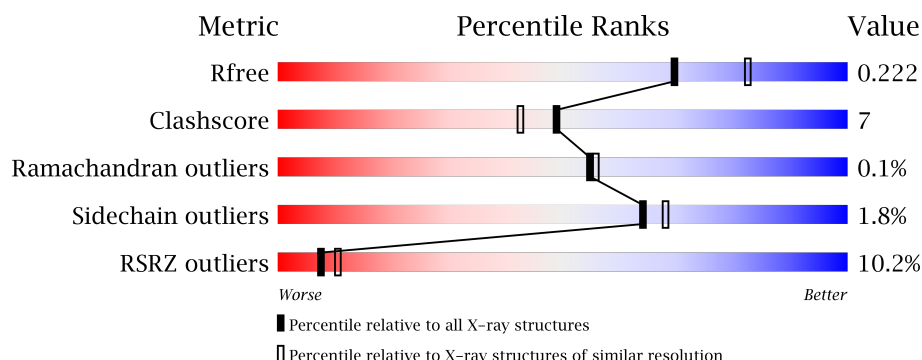
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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. 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>7%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	535	<div> <div>19%</div> <div>85%</div> <div>14%</div> <div>..</div> </div>
2	B	256	<div> <div>3%</div> <div>95%</div> <div>.</div> </div>
2	D	256	<div> <div>5%</div> <div>93%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	HTH	B	286	-	-	-	X
3	OH	A	802	-	-	-	X
4	DMU	A	1005	-	-	-	X
4	DMU	B	2	-	-	-	X
4	DMU	B	3	-	-	-	X
4	DMU	C	10	-	-	-	X
4	DMU	C	9	-	-	-	X
5	TRD	A	1013	-	-	-	X
5	TRD	A	3	-	-	-	X
5	TRD	B	4	-	-	-	X
5	TRD	D	3	-	-	-	X
6	HEA	A	1	X	-	-	-
6	HEA	A	2[A]	X	-	-	-
6	HEA	A	2[B]	X	-	-	-
6	HEA	C	1	X	-	-	-
6	HEA	C	2[A]	X	-	-	-
6	HEA	C	2[B]	X	-	-	-
8	MG	A	6	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13755 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	13	0
			4274	2862	673	707	32			
1	C	531	Total	C	N	O	S	0	13	0
			4219	2826	663	698	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	ASP	ENGINEERED MUTATION	UNP Q3J5A7
C	132	ALA	ASP	ENGINEERED MUTATION	UNP Q3J5A7

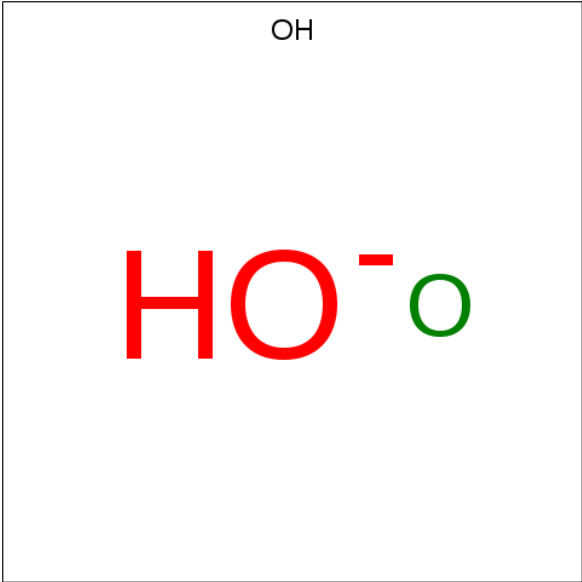
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2021	1319	333	363	6			
2	D	256	Total	C	N	O	S	0	0	0
			2015	1316	330	363	6			

There are 8 discrepancies between the modelled and reference sequences:

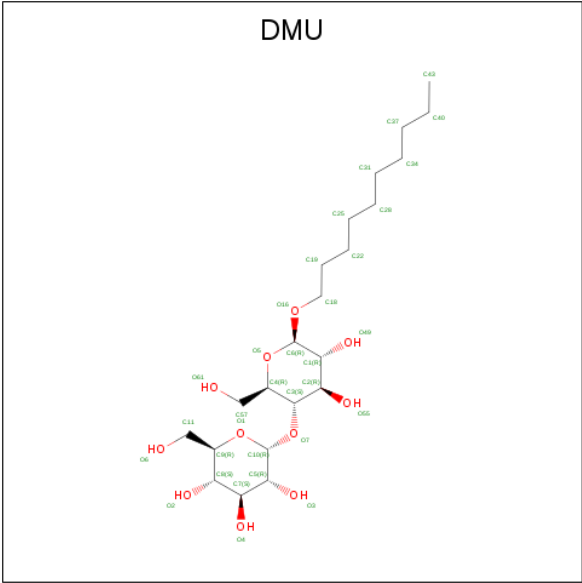
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	284	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	285	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	284	HIS	-	EXPRESSION TAG	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 DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



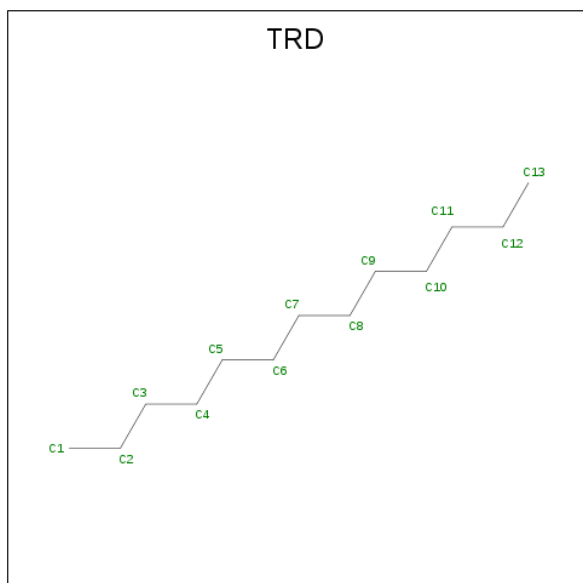
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			22	16 6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	16	5		
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
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			33	22	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:  $C_{13}H_{28}$ ).



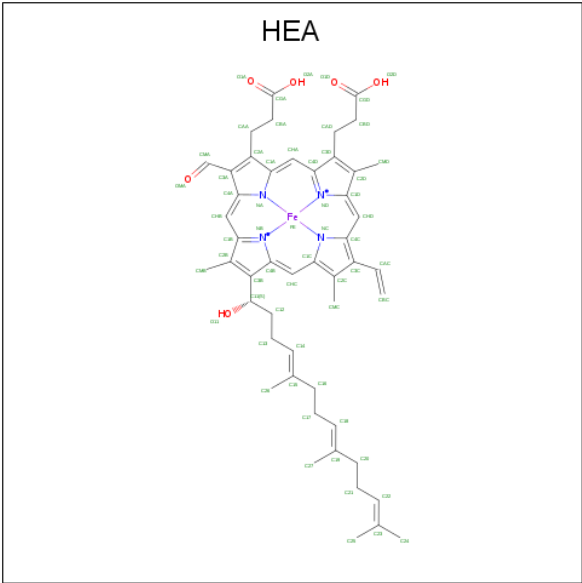
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			7	7		
5	A	1	Total	C	0	0
			6	6		
5	A	1	Total	C	0	0
			13	13		
5	A	1	Total	C	0	0
			13	13		
5	B	1	Total	C	0	0
			8	8		
5	C	1	Total	C	0	0
			13	13		
5	D	1	Total	C	0	0
			13	13		
5	D	1	Total	C	0	0
			7	7		

- Molecule 6 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
6	A	1	Total 120	C 98	Fe 2	N 8	O 12	0	1
6	C	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	Fe	N	O	0	1
			120	98	2	8	12		

- Molecule 7 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Cu	0	0
			2	2		
7	A	1	Total	Cu	0	0
			1	1		
7	D	2	Total	Cu	0	0
			2	2		
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).

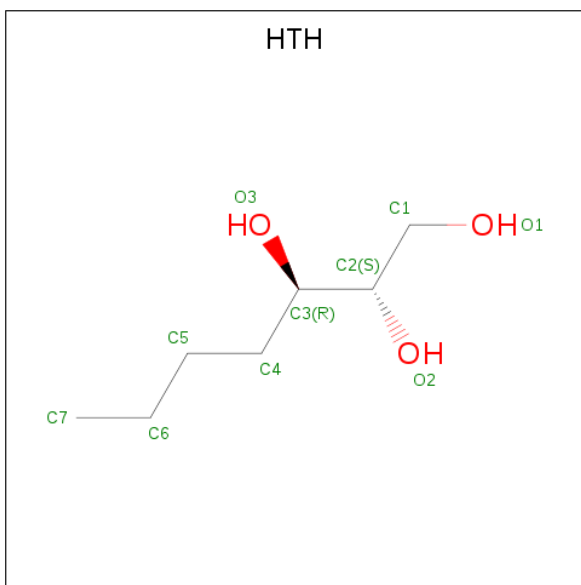
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		
10	C	1	Total	Cl	0	0
			1	1		

- Molecule 11 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).





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

- 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		

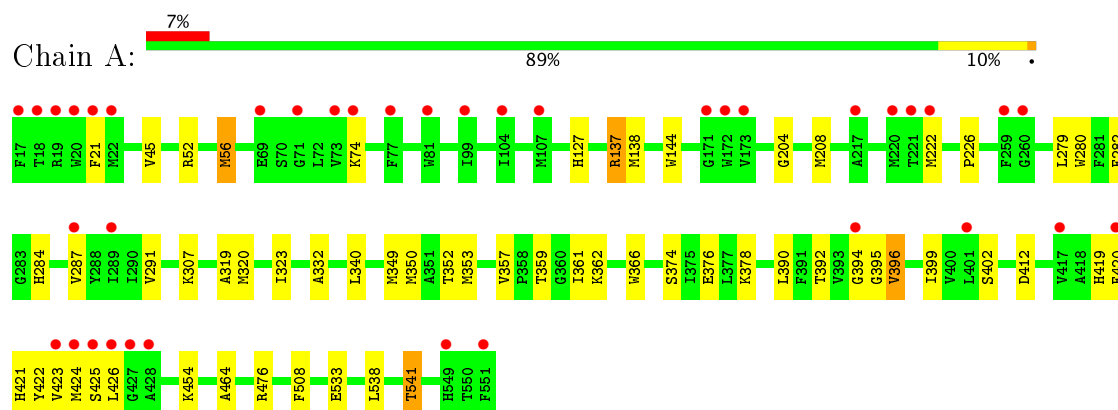
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	132	Total	O	0	1
			133	133		
13	B	128	Total	O	0	0
			128	128		
13	C	88	Total	O	0	0
			88	88		
13	D	112	Total	O	0	0
			112	112		

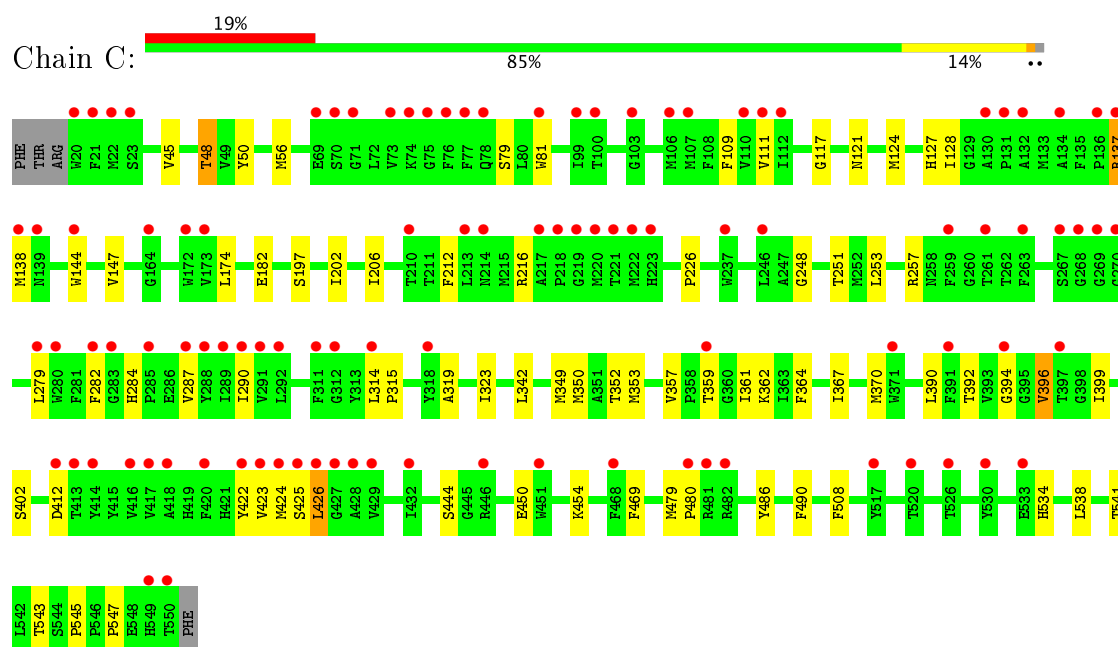
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Cytochrome c oxidase, aa3 type, subunit I

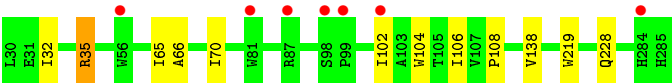


- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

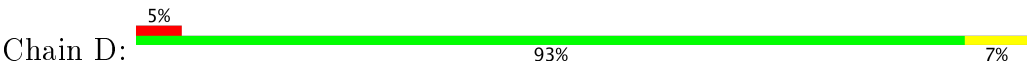


- Molecule 2: Cytochrome c oxidase subunit 2





● 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, $\alpha$ , $\beta$ , $\gamma$	124.67Å 132.03Å 176.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 2.15 42.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.70-2.15) 97.2 (42.70-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.198 , 0.219 0.200 , 0.222	Depositor DCC
$R_{free}$ test set	4627 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 74.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [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, CL, TRD, CD, DMU, HTH, 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	0.54	0/4430	0.55	0/6048
1	C	0.46	0/4373	0.53	0/5973
2	B	0.50	0/2083	0.56	0/2852
2	D	0.46	0/2077	0.52	0/2845
All	All	0.49	0/12963	0.54	0/17718

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	4274	0	4182	68	0
1	C	4219	0	4120	87	0
2	B	2021	0	1978	10	0
2	D	2015	0	1967	14	0
3	A	1	0	0	1	0
3	C	1	0	0	1	0
4	A	43	0	61	2	0
4	B	122	0	147	0	0
4	C	79	0	84	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	46	0	42	1	0
5	A	46	0	90	2	0
5	B	8	0	12	0	0
5	C	13	0	28	1	0
5	D	20	0	41	0	0
6	A	180	0	162	19	0
6	C	180	0	162	21	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	2	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	A	1	0	0	0	0
10	C	1	0	0	0	0
11	B	10	0	16	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	A	133	0	0	2	0
13	B	128	0	0	2	0
13	C	88	0	0	2	0
13	D	112	0	0	1	0
All	All	13755	0	13092	180	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 7.

The worst 5 of 180 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:137:ARG:HG3	1:A:137:ARG:HH11	1.03	1.17
1:A:357:VAL:O	1:A:361[B]:ILE:HG12	1.52	1.07
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:HG	1.41	1.00
1:C:422[A]:TYR:CD2	1:C:426[A]:LEU:HD12	1.97	0.99
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.30	0.93

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	546/535 (102%)	533 (98%)	13 (2%)	0	100	100
1	C	542/535 (101%)	526 (97%)	16 (3%)	0	100	100
2	B	254/256 (99%)	246 (97%)	8 (3%)	0	100	100
2	D	254/256 (99%)	248 (98%)	5 (2%)	1 (0%)	38	32
All	All	1596/1582 (101%)	1553 (97%)	42 (3%)	1 (0%)	55	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	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	437/434 (101%)	427 (98%)	10 (2%)	56	59
1	C	430/434 (99%)	421 (98%)	9 (2%)	59	62
2	B	214/215 (100%)	212 (99%)	2 (1%)	82	87
2	D	213/215 (99%)	210 (99%)	3 (1%)	71	77
All	All	1294/1298 (100%)	1270 (98%)	24 (2%)	64	66

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	35	ARG
1	C	137	ARG
2	D	104	TRP
2	B	104	TRP
1	C	48	THR

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 45 ligands modelled in this entry, 2 are modelled with single atom and 16 are monoatomic - leaving 27 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	44,67,67	1.40	3 (6%)	37,103,103	1.60	9 (24%)
4	DMU	A	1005	-	22,22,34	0.55	0	27,27,45	0.94	1 (3%)
5	TRD	A	1009	-	6,6,12	0.25	0	5,5,11	0.37	0
5	TRD	A	1013	-	6,6,12	0.24	0	5,5,11	0.45	0
6	HEA	A	2[A]	1,13	44,67,67	1.41	5 (11%)	37,103,103	1.61	8 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	HEA	A	2[B]	1,13	44,67,67	1.41	4 (9%)	37,103,103	1.54	10 (27%)
5	TRD	A	3	-	12,12,12	0.28	0	11,11,11	0.51	0
5	TRD	A	552	-	5,5,12	0.31	0	4,4,11	0.31	0
5	TRD	A	553	-	12,12,12	0.24	0	11,11,11	0.52	0
4	DMU	A	7	-	21,21,34	0.59	0	25,25,45	1.05	2 (8%)
4	DMU	B	1	-	34,34,34	0.50	0	45,45,45	0.92	2 (4%)
4	DMU	B	2	-	34,34,34	0.53	0	45,45,45	0.78	1 (2%)
11	HTH	B	286	-	9,9,9	0.39	0	9,10,10	0.86	0
4	DMU	B	3	-	34,34,34	0.56	0	45,45,45	0.61	0
5	TRD	B	4	-	7,7,12	0.25	0	6,6,11	0.40	0
4	DMU	B	6	-	24,24,34	0.55	0	35,35,45	0.72	0
6	HEA	C	1	1	44,67,67	1.38	6 (13%)	37,103,103	1.58	9 (24%)
4	DMU	C	10	-	34,34,34	0.60	0	45,45,45	0.83	1 (2%)
6	HEA	C	2[A]	1,13	44,67,67	1.41	5 (11%)	37,103,103	1.52	8 (21%)
6	HEA	C	2[B]	1,13	44,67,67	1.42	3 (6%)	37,103,103	1.48	7 (18%)
4	DMU	C	5	-	24,24,34	0.53	0	35,35,45	0.65	0
5	TRD	C	552	-	12,12,12	0.23	0	11,11,11	0.55	0
4	DMU	C	9	-	24,24,34	0.59	0	35,35,45	0.92	2 (5%)
5	TRD	D	14	-	6,6,12	0.24	0	5,5,11	0.35	0
5	TRD	D	3	-	12,12,12	0.19	0	11,11,11	0.65	0
4	DMU	D	4	-	24,24,34	0.52	0	35,35,45	0.65	0
4	DMU	D	8	-	24,24,34	0.54	0	35,35,45	0.64	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
6	HEA	A	2[A]	1,13	3/3/7/16	0/24/76/76	0/0/8/8
6	HEA	A	2[B]	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	-	-	0/3/3/10	0/0/0/0
5	TRD	A	553	-	-	0/10/10/10	0/0/0/0
4	DMU	A	7	-	-	0/13/29/59	0/1/1/2
4	DMU	B	1	-	-	0/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMU	B	2	-	-	0/19/59/59	0/2/2/2
11	HTH	B	286	-	-	0/10/10/10	0/0/0/0
4	DMU	B	3	-	-	0/19/59/59	0/2/2/2
5	TRD	B	4	-	-	0/5/5/10	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[A]	1,13	3/3/7/16	0/24/76/76	0/0/8/8
6	HEA	C	2[B]	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 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	HEA	C3A-C2A	-4.92	1.33	1.40
6	C	2[B]	HEA	C3A-C2A	-4.76	1.34	1.40
6	A	2[B]	HEA	C3A-C2A	-4.72	1.34	1.40
6	A	2[A]	HEA	C3A-C2A	-4.64	1.34	1.40
6	C	1	HEA	C3A-C2A	-4.31	1.34	1.40

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2[A]	HEA	CAD-CBD-CGD	-5.01	104.10	112.66
6	C	2[A]	HEA	CAD-CBD-CGD	-4.00	105.83	112.66
6	C	1	HEA	CMC-C2C-C1C	-3.63	122.88	128.46
6	C	1	HEA	CMB-C2B-C1B	-2.97	123.91	128.46
6	A	1	HEA	CMB-C2B-C1B	-2.86	124.06	128.46

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	2[A]	HEA	NB
6	C	2[A]	HEA	NA
6	C	2[A]	HEA	ND

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Mol	Chain	Res	Type	Atom
6	C	2[B]	HEA	ND
6	C	2[B]	HEA	NA

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1	HEA	3	0
4	A	1005	DMU	2	0
6	A	2[A]	HEA	7	0
6	A	2[B]	HEA	9	0
5	A	3	TRD	1	0
5	A	553	TRD	1	0
6	C	1	HEA	6	0
4	C	10	DMU	1	0
6	C	2[A]	HEA	7	0
6	C	2[B]	HEA	8	0
5	C	552	TRD	1	0
4	C	9	DMU	1	0
4	D	8	DMU	1	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, 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	535/535 (100%)	0.15	38 (7%) 17 22	24, 35, 57, 81	0
1	C	531/535 (99%)	0.78	102 (19%) 1 2	30, 52, 76, 88	0
2	B	256/256 (100%)	-0.16	7 (2%) 55 63	23, 39, 55, 59	0
2	D	256/256 (100%)	0.03	14 (5%) 26 33	30, 44, 64, 72	0
All	All	1578/1582 (99%)	0.29	161 (10%) 7 10	23, 42, 67, 88	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	7.2
2	D	284	HIS	6.9
1	C	222	MET	6.7
2	B	56	TRP	6.0
1	A	20	TRP	5.8

### 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMU	C	9	23/33	0.50	0.36	8.70	85,86,89,89	23
4	DMU	B	2	33/33	0.88	0.16	8.39	49,54,56,57	33
5	TRD	B	4	8/13	0.87	0.31	5.57	35,36,37,37	0
11	HTH	B	286	10/10	0.80	0.33	4.57	56,60,61,61	0
5	TRD	A	1013	7/13	0.68	0.26	4.05	54,56,57,57	0
4	DMU	A	1005	22/33	0.79	0.14	4.02	44,49,53,54	22
5	TRD	A	3	13/13	0.84	0.28	3.47	46,49,53,54	0
4	DMU	C	10	33/33	0.87	0.18	3.30	73,74,76,76	0
8	MG	A	6	1/1	0.99	0.22	3.21	13,13,13,13	0
4	DMU	B	3	33/33	0.88	0.27	2.92	73,78,82,83	0
5	TRD	D	3	13/13	0.85	0.29	2.66	55,58,61,61	0
3	OH	A	802	1/1	0.98	0.30	2.44	8,8,8,8	1
8	MG	C	6	1/1	0.99	0.24	1.58	18,18,18,18	0
4	DMU	B	1	33/33	0.94	0.11	1.54	26,35,46,48	0
5	TRD	D	14	7/13	0.77	0.16	1.27	65,65,65,65	0
4	DMU	A	7	21/33	0.80	0.18	1.05	43,59,70,72	0
6	HEA	A	2[B]	60/60	0.96	0.24	0.92	30,33,41,41	60
6	HEA	A	2[A]	60/60	0.96	0.24	0.78	21,22,30,32	60
5	TRD	A	1009	7/13	0.84	0.15	0.74	57,58,58,58	0
6	HEA	A	1	60/60	0.98	0.20	0.32	21,25,30,32	0
6	HEA	C	2[B]	60/60	0.96	0.21	0.16	35,40,48,48	60
6	HEA	C	1	60/60	0.96	0.22	0.13	31,34,47,47	0
9	CA	A	554	1/1	1.00	0.09	0.11	27,27,27,27	0
6	HEA	C	2[A]	60/60	0.96	0.21	-0.01	25,28,33,34	60
7	CU1	B	288	1/1	1.00	0.12	-0.01	26,26,26,26	0
7	CU1	D	287	1/1	1.00	0.11	-0.43	32,32,32,32	0
12	CD	B	9	1/1	0.99	0.13	-0.49	39,39,39,39	1
7	CU1	D	286	1/1	1.00	0.12	-0.57	33,33,33,33	0
7	CU1	B	287	1/1	1.00	0.10	-1.17	25,25,25,25	0
12	CD	D	288	1/1	0.99	0.07	-1.40	40,40,40,40	0
10	CL	C	554	1/1	0.89	0.18	-2.11	68,68,68,68	0
12	CD	B	8	1/1	0.99	0.07	-2.43	41,41,41,41	0
10	CL	A	10	1/1	0.97	0.04	-2.88	41,41,41,41	0
12	CD	D	9	1/1	0.96	0.07	-3.23	63,63,63,63	1
9	CA	C	7	1/1	0.98	0.04	-3.58	38,38,38,38	0
4	DMU	D	4	23/33	0.86	0.23	-	91,91,91,91	23
3	OH	C	802	1/1	0.97	0.84	-	21,21,21,21	1
5	TRD	C	552	13/13	0.75	0.19	-	80,82,83,84	0
4	DMU	C	5	23/33	0.80	0.24	-	97,98,98,99	23
4	DMU	D	8	23/33	0.78	0.23	-	89,90,93,93	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CU1	C	553	1/1	0.98	0.15	-	45,45,45,45	0
7	CU1	A	5	1/1	0.99	0.17	-	37,37,37,37	0
4	DMU	B	6	23/33	0.81	0.19	-	76,77,78,78	23
5	TRD	A	552	6/13	0.75	0.18	-	62,63,63,63	0
5	TRD	A	553	13/13	0.78	0.25	-	71,71,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.