



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 05:14 PM GMT

PDB ID : 3DTU
Title : Catalytic core subunits (I and II) of cytochrome c oxidase from Rhodobacter sphaeroides complexed with deoxycholic acid
Authors : Qin, L.; Mills, D.A.; Buhrow, L.; Hiser, C.; Ferguson-Miller, S.
Deposited on : 2008-07-15
Resolution : 2.15 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

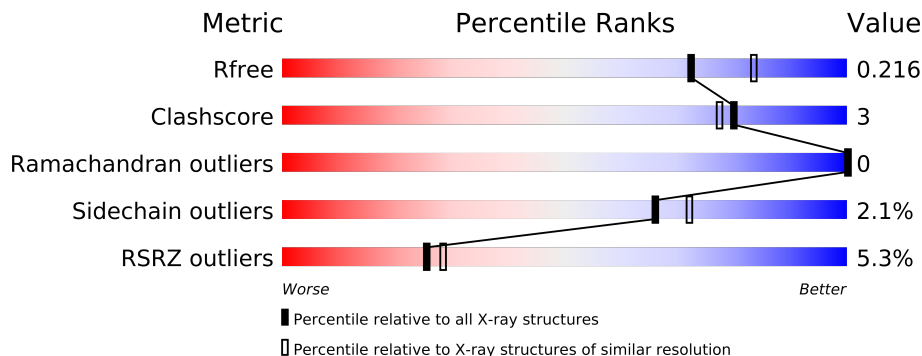
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	566	
1	C	566	
2	B	262	
2	D	262	

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

Mol	Type	Chain	Res	Geometry	Electron density
10	TRD	A	1009	-	X
10	TRD	A	1010	-	X
10	TRD	A	1013	-	X
10	TRD	A	1014	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
10	TRD	A	1015	-	X
10	TRD	B	1012	-	X
10	TRD	B	1031	-	X
10	TRD	C	578	-	X
10	TRD	C	579	-	X
10	TRD	C	580	-	X
10	TRD	C	581	-	X
10	TRD	C	582	-	X
10	TRD	C	583	-	X
10	TRD	C	584	-	X
10	TRD	D	12	-	X
10	TRD	D	23	-	X
10	TRD	D	288	-	X
12	HTO	B	1	-	X
13	DXC	C	576	-	X
3	DMU	A	1004	-	X
3	DMU	A	1005	-	X
3	DMU	B	1003	-	X
3	DMU	C	567	-	X
3	DMU	C	568	-	X
3	DMU	D	11	-	X
8	PO4	A	1001	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 13976 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	33	0	0
			4249	2845	673	700	31			
1	C	536	Total	C	N	O	S	32	0	0
			4221	2827	664	699	31			

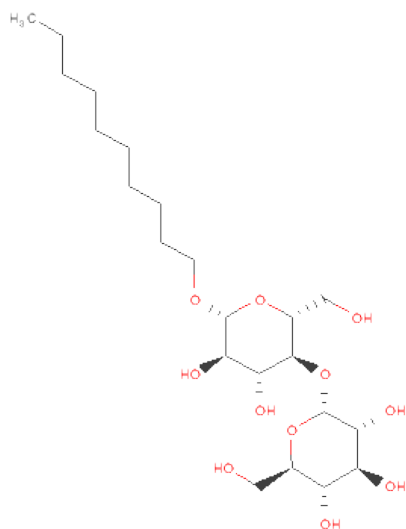
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	21	0	0
			2051	1336	340	369	6			
2	D	258	Total	C	N	O	S	15	0	0
			2040	1329	336	369	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	EXPRESSION TAG	UNP Q03736
B	283	HIS	-	EXPRESSION TAG	UNP Q03736
B	284	HIS	-	EXPRESSION TAG	UNP Q03736
B	285	HIS	-	EXPRESSION TAG	UNP Q03736
B	286	HIS	-	EXPRESSION TAG	UNP Q03736
B	287	HIS	-	EXPRESSION TAG	UNP Q03736
D	282	HIS	-	EXPRESSION TAG	UNP Q03736
D	283	HIS	-	EXPRESSION TAG	UNP Q03736
D	284	HIS	-	EXPRESSION TAG	UNP Q03736
D	285	HIS	-	EXPRESSION TAG	UNP Q03736
D	286	HIS	-	EXPRESSION TAG	UNP Q03736
D	287	HIS	-	EXPRESSION TAG	UNP Q03736

- Molecule 3 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			33	22	11		
3	A	1	Total	C	O	0	0
			22	11	11		
3	A	1	Total	C	O	0	0
			22	16	6		
3	A	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			23	17	6		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			33	22	11		
3	C	1	Total	C	O	0	0
			33	22	11		
3	D	1	Total	C	O	0	0
			33	22	11		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cu	0	0
			2	2		
4	A	1	Total	Cu	0	0
			1	1		
4	D	2	Total	Cu	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cu 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

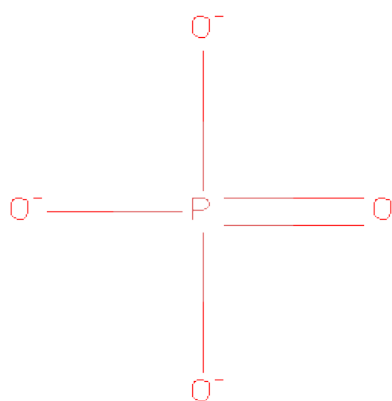
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0

- Molecule 7 is HYDROXIDE ION (three-letter code: OH) (formula: HO).

HO⁻

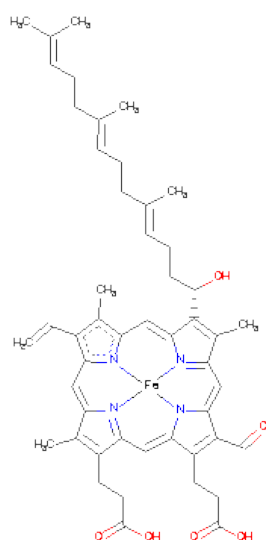
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	O	P		0	0
			5	4	1			
8	C	1	Total	O	P		0	0
			5	4	1			

- Molecule 9 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



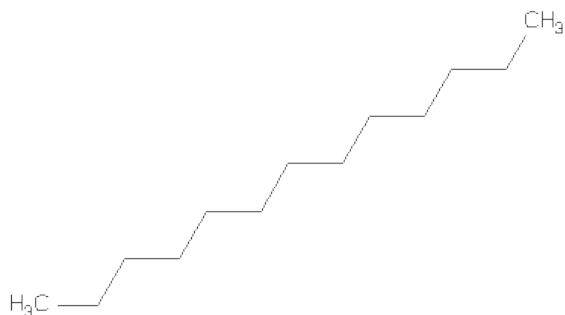
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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

- Molecule 10 is TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	C		
			13	13	0	0
10	A	1	Total	C		
			11	11	0	0
10	A	1	Total	C		
			13	13	0	0
10	A	1	Total	C		
			7	7	0	0
10	A	1	Total	C		
			11	11	0	0
10	A	1	Total	C		
			7	7	0	0
10	A	1	Total	C		
			7	7	0	0
10	A	1	Total	C		
			11	11	0	0

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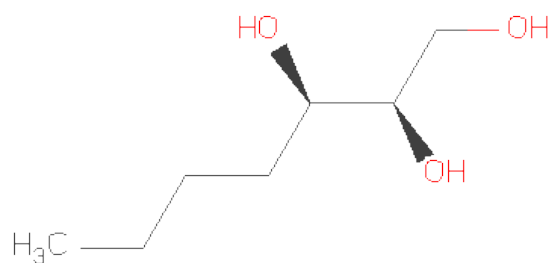
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 9 9	0	0
10	B	1	Total C 9 9	0	0
10	B	1	Total C 9 9	0	0
10	C	1	Total C 13 13	0	0
10	C	1	Total C 11 11	0	0
10	C	1	Total C 7 7	0	0
10	C	1	Total C 9 9	0	0
10	C	1	Total C 11 11	0	0
10	C	1	Total C 7 7	0	0
10	C	1	Total C 7 7	0	0
10	C	1	Total C 7 7	0	0
10	D	1	Total C 13 13	0	0
10	D	1	Total C 9 9	0	0
10	D	1	Total C 11 11	0	0
10	D	1	Total C 7 7	0	0

- Molecule 11 is CADMIUM ION (three-letter code: CD) (formula: Cd).

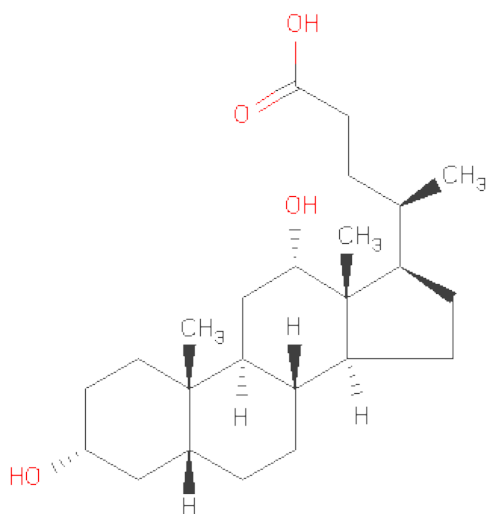
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	3	Total Cd 3 3	0	0
11	D	2	Total Cd 2 2	0	0

- Molecule 12 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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

- Molecule 13 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OICACID (three-letter code: DXC) (formula: C₂₄H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			28	24	4		

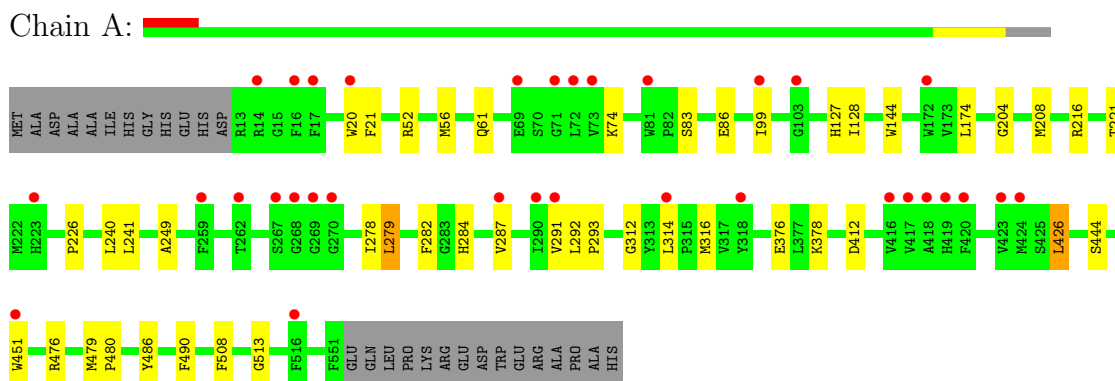
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	144	Total 144	O 144	0	0
14	B	160	Total 160	O 160	0	0
14	C	169	Total 169	O 169	0	0
14	D	163	Total 163	O 163	0	0

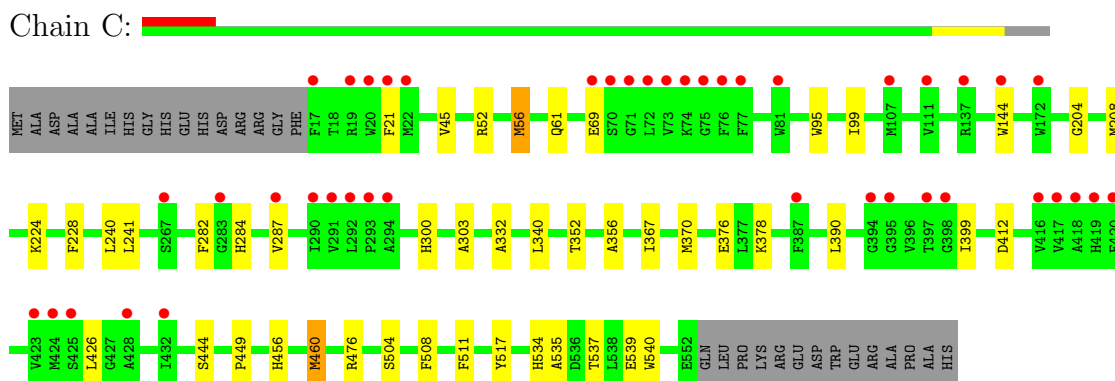
3 Residue-property plots

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

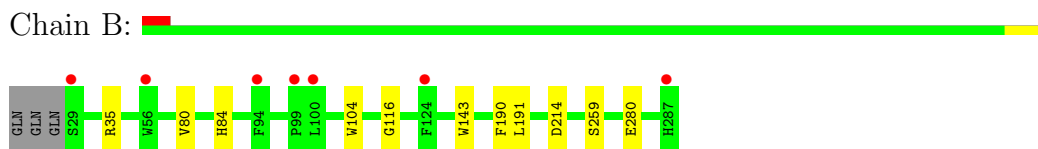
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1



• 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	123.24Å 132.05Å 167.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.15 39.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.00-2.15) 96.9 (39.90-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.212 0.185 , 0.216	Depositor DCC
R_{free} test set	3612 reflections (2.57%)	DCC
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 144361 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13976	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OH, HTO, PO4, TRD, CD, HEA, DXC, CA, CU, DMU

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	0.50	0/4406	0.55	2/6010 (0.0%)
1	C	0.53	0/4377	0.56	0/5973
2	B	0.48	0/2115	0.54	0/2895
2	D	0.53	0/2102	0.57	0/2877
All	All	0.51	0/13000	0.56	2/17755 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	279	LEU	CA-CB-CG	-5.14	103.48	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4249	0	4172	30	0
1	C	4221	0	4140	39	1
2	B	2051	0	2001	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2040	0	1995	6	1
3	A	110	0	131	10	0
3	B	46	0	52	0	0
3	C	66	0	84	1	0
3	D	33	0	42	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	1	0
7	C	1	0	0	1	0
8	A	5	0	0	0	0
8	C	5	0	0	0	0
9	A	120	0	108	5	0
9	C	120	0	108	8	0
10	A	80	0	158	7	0
10	B	27	0	51	1	0
10	C	72	0	139	13	0
10	D	40	0	79	2	0
11	B	3	0	0	0	0
11	D	2	0	0	0	0
12	B	10	0	16	1	0
13	C	28	0	39	0	0
14	A	144	0	0	1	0
14	B	160	0	0	0	0
14	C	169	0	0	3	0
14	D	163	0	0	1	0
All	All	13976	0	13315	91	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 91 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:303:ALA:HB3	10:C:584:TRD:H21	1.38	1.05
3:A:1002:DMU:C2	3:A:1002:DMU:C6	2.49	0.90
7:C:572:OH:O	14:C:589:HOH:O	1.89	0.90
9:C:574:HEA:HBC1	9:C:574:HEA:HMC1	1.59	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:1501:OH:O	14:A:1511:HOH:O	2.00	0.79

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:GLU:OE1	2:D:86:LYS:NZ[4.444]	1.87	0.33

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	537/566 (95%)	525 (98%)	12 (2%)	0	100	100
1	C	534/566 (94%)	526 (98%)	8 (2%)	0	100	100
2	B	257/262 (98%)	250 (97%)	7 (3%)	0	100	100
2	D	256/262 (98%)	251 (98%)	5 (2%)	0	100	100
All	All	1584/1656 (96%)	1552 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	438/459 (95%)	426 (97%)	12 (3%)	57	60
1	C	436/459 (95%)	427 (98%)	9 (2%)	66	72
2	B	218/221 (99%)	215 (99%)	3 (1%)	78	86
2	D	217/221 (98%)	213 (98%)	4 (2%)	71	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1309/1360 (96%)	1281 (98%)	28 (2%)	66 72

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

Mol	Chain	Res	Type
2	B	35	ARG
1	C	52	ARG
2	D	35	ARG
2	B	104	TRP
2	B	214	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	228	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 2 are modelled with single atom and 15 are monoatomic - leaving 40 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$
8	PO4	A	1001	-	4,4,4	0.31	0	6,6,6	0.31	0
3	DMU	A	1002	-	19,21,34	3.57	1 (5%)	23,28,45	1.13	2 (8%)
3	DMU	A	1004	-	22,22,34	0.62	0	27,27,45	0.98	1 (3%)
3	DMU	A	1005	-	34,34,34	0.59	0	45,45,45	0.68	0
10	TRD	A	1009	-	6,6,12	3.15	1 (16%)	5,5,11	0.58	0
10	TRD	A	1010	-	10,10,12	1.65	1 (10%)	9,9,11	0.67	0
10	TRD	A	1013	-	6,6,12	3.13	1 (16%)	5,5,11	0.49	0
10	TRD	A	1014	-	6,6,12	3.51	1 (16%)	5,5,11	0.80	0
10	TRD	A	1015	-	10,10,12	1.59	1 (10%)	9,9,11	0.62	0
9	HEA	A	1502	1	67,67,67	1.73	10 (14%)	80,103,103	1.35	11 (13%)
9	HEA	A	1503	1,14	67,67,67	1.95	12 (17%)	80,103,103	1.60	16 (20%)
10	TRD	A	1504	-	12,12,12	0.29	0	11,11,11	0.45	0
10	TRD	A	1505	-	10,10,12	1.71	1 (10%)	9,9,11	0.64	0
10	TRD	A	1506	-	12,12,12	0.26	0	11,11,11	0.51	0
3	DMU	A	567	-	34,34,34	0.55	0	45,45,45	0.78	1 (2%)
12	HTO	B	1	-	9,9,9	0.22	0	10,10,10	0.77	0
3	DMU	B	1003	-	22,23,34	0.51	0	27,28,45	0.73	0
3	DMU	B	1011	-	24,24,34	0.76	1 (4%)	34,35,45	0.72	0
10	TRD	B	1012	-	8,8,12	2.82	1 (12%)	7,7,11	0.73	0
10	TRD	B	1023	-	8,8,12	2.83	1 (12%)	7,7,11	0.59	0
10	TRD	B	1031	-	8,8,12	2.97	1 (12%)	7,7,11	0.70	0
3	DMU	C	567	-	34,34,34	0.64	0	45,45,45	0.77	2 (4%)
3	DMU	C	568	-	34,34,34	0.57	0	45,45,45	0.83	2 (4%)
8	PO4	C	573	-	4,4,4	0.29	0	6,6,6	0.30	0
9	HEA	C	574	1	67,67,67	1.75	8 (11%)	80,103,103	1.22	7 (8%)
9	HEA	C	575	1,14	67,67,67	1.89	12 (17%)	80,103,103	1.49	14 (17%)
13	DXC	C	576	11	31,31,31	0.54	0	49,49,49	1.22	6 (12%)
10	TRD	C	577	-	12,12,12	0.30	0	11,11,11	0.41	0
10	TRD	C	578	-	10,10,12	1.86	1 (10%)	9,9,11	0.51	0
10	TRD	C	579	-	6,6,12	3.10	1 (16%)	5,5,11	0.54	0
10	TRD	C	580	-	8,8,12	2.97	1 (12%)	7,7,11	0.65	0
10	TRD	C	581	-	10,10,12	1.73	1 (10%)	9,9,11	0.66	0
10	TRD	C	582	-	6,6,12	3.23	1 (16%)	5,5,11	0.60	0
10	TRD	C	583	-	6,6,12	3.50	1 (16%)	5,5,11	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	TRD	C	584	-	6,6,12	4.64	1 (16%)	5,5,11	0.71	0
3	DMU	D	11	-	34,34,34	0.55	0	45,45,45	0.82	1 (2%)
10	TRD	D	12	-	10,10,12	2.06	1 (10%)	9,9,11	0.73	0
10	TRD	D	23	-	6,6,12	3.39	1 (16%)	5,5,11	0.83	0
10	TRD	D	288	-	8,8,12	2.79	1 (12%)	7,7,11	0.61	0
10	TRD	D	7	-	12,12,12	0.26	0	11,11,11	0.56	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
8	PO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	DMU	A	1002	-	-	0/14/37/59	0/1/1/2
3	DMU	A	1004	-	-	0/13/33/59	0/1/1/2
3	DMU	A	1005	-	-	0/19/59/59	0/2/2/2
10	TRD	A	1009	-	-	0/4/4/10	0/0/0/0
10	TRD	A	1010	-	-	0/8/8/10	0/0/0/0
10	TRD	A	1013	-	-	0/4/4/10	0/0/0/0
10	TRD	A	1014	-	-	0/4/4/10	0/0/0/0
10	TRD	A	1015	-	-	0/8/8/10	0/0/0/0
9	HEA	A	1502	1	-	0/30/76/76	0/0/8/8
9	HEA	A	1503	1,14	-	0/30/76/76	0/0/8/8
10	TRD	A	1504	-	-	0/10/10/10	0/0/0/0
10	TRD	A	1505	-	-	0/8/8/10	0/0/0/0
10	TRD	A	1506	-	-	0/10/10/10	0/0/0/0
3	DMU	A	567	-	-	0/19/59/59	0/2/2/2
12	HTO	B	1	-	1/1/2/2	0/10/10/10	0/0/0/0
3	DMU	B	1003	-	-	0/15/35/59	0/1/1/2
3	DMU	B	1011	-	-	0/8/48/59	0/2/2/2
10	TRD	B	1012	-	-	0/6/6/10	0/0/0/0
10	TRD	B	1023	-	-	0/6/6/10	0/0/0/0
10	TRD	B	1031	-	-	0/6/6/10	0/0/0/0
3	DMU	C	567	-	-	0/19/59/59	0/2/2/2
3	DMU	C	568	-	-	0/19/59/59	0/2/2/2
8	PO4	C	573	-	-	0/0/0/0	0/0/0/0
9	HEA	C	574	1	-	0/30/76/76	0/0/8/8
9	HEA	C	575	1,14	-	0/30/76/76	0/0/8/8
13	DXC	C	576	11	-	0/9/71/71	0/0/4/4
10	TRD	C	577	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	TRD	C	578	-	-	0/8/8/10	0/0/0/0
10	TRD	C	579	-	-	0/4/4/10	0/0/0/0
10	TRD	C	580	-	-	0/6/6/10	0/0/0/0
10	TRD	C	581	-	-	0/8/8/10	0/0/0/0
10	TRD	C	582	-	-	0/4/4/10	0/0/0/0
10	TRD	C	583	-	-	0/4/4/10	0/0/0/0
10	TRD	C	584	-	-	0/4/4/10	0/0/0/0
3	DMU	D	11	-	-	0/19/59/59	0/2/2/2
10	TRD	D	12	-	-	0/8/8/10	0/0/0/0
10	TRD	D	23	-	-	0/4/4/10	0/0/0/0
10	TRD	D	288	-	-	0/6/6/10	0/0/0/0
10	TRD	D	7	-	-	0/10/10/10	0/0/0/0

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	DMU	O55-C2	15.35	1.42	1.25
10	C	584	TRD	C7-C6	-11.36	1.50	1.55
10	A	1014	TRD	C7-C6	-8.58	1.51	1.55
10	C	583	TRD	C7-C6	-8.57	1.51	1.55
10	C	580	TRD	C9-C8	-8.38	1.51	1.55

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1503	HEA	C2A-C1A-NA	-3.96	106.67	109.64
9	A	1503	HEA	C3A-C4A-NA	-3.91	105.88	111.52
9	C	575	HEA	CAD-CBD-CGD	-3.87	101.03	113.47
3	A	1002	DMU	O7-C3-C4	3.77	110.92	104.84
9	A	1502	HEA	C4A-CHB-C1B	-3.74	122.55	127.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	1	HTO	C2

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	539/566 (95%)	0.17	33 (6%) 21 24	26, 37, 60, 76	7 (1%)
1	C	536/566 (94%)	0.20	43 (8%) 12 15	22, 33, 49, 67	7 (1%)
2	B	259/262 (98%)	-0.15	7 (2%) 52 56	26, 38, 52, 65	5 (1%)
2	D	258/262 (98%)	-0.25	4 (1%) 68 75	24, 35, 46, 57	4 (1%)
All	All	1592/1656 (96%)	0.06	87 (5%) 25 27	22, 35, 52, 76	23 (1%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	7.7
1	C	73	VAL	6.6
1	C	17	PHE	5.4
1	A	81	TRP	5.3
1	C	21	PHE	5.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	TRD	A	1009	7/13	0.35	17.63	60,60,62,62	0
10	TRD	C	584	7/13	0.39	11.57	46,50,54,55	0
10	TRD	C	581	11/13	0.36	10.74	74,75,77,77	11
3	DMU	C	567	33/33	0.47	9.42	77,81,82,83	0
10	TRD	B	1012	9/13	0.24	8.77	74,75,77,77	0
10	TRD	C	582	7/13	0.28	8.66	67,67,67,67	7
10	TRD	A	1014	7/13	0.34	6.34	73,73,74,74	7
3	DMU	A	1005	33/33	0.26	6.26	50,57,61,61	33
10	TRD	D	12	11/13	0.24	6.24	58,58,58,59	11
10	TRD	C	578	11/13	0.23	6.21	61,62,63,63	0
3	DMU	D	11	33/33	0.26	5.14	70,73,74,75	33
10	TRD	D	23	7/13	0.21	4.14	61,61,62,62	7
3	DMU	B	1003	23/33	0.41	4.07	49,54,56,56	23
10	TRD	B	1031	9/13	0.24	3.61	53,55,58,58	0
10	TRD	C	580	9/13	0.26	3.50	62,64,64,64	9
10	TRD	A	1013	7/13	0.26	3.45	53,54,55,55	0
8	PO4	A	1001	5/5	0.28	3.40	69,69,70,70	5
12	HTO	B	1	10/10	0.23	3.16	51,54,55,56	0
10	TRD	D	288	9/13	0.19	3.10	52,53,56,56	0
3	DMU	C	568	33/33	0.20	2.97	65,68,69,70	0
10	TRD	C	579	7/13	0.34	2.94	68,68,69,69	0
10	TRD	C	583	7/13	0.21	2.85	57,57,59,59	0
3	DMU	A	1004	22/33	0.21	2.71	44,61,65,66	22
10	TRD	A	1010	11/13	0.19	2.66	58,59,59,60	11
13	DXC	C	576	28/28	0.18	2.31	46,50,52,52	0
10	TRD	A	1015	11/13	0.19	2.09	63,65,70,70	11
10	TRD	A	1504	13/13	0.22	1.31	56,58,61,62	0
8	PO4	C	573	5/5	0.29	1.31	53,53,54,55	5
3	DMU	A	567	33/33	0.15	1.12	48,63,67,68	0
5	MG	C	570	1/1	0.18	0.95	15,15,15,15	0
10	TRD	A	1506	13/13	0.14	0.78	45,46,51,53	0
10	TRD	A	1505	11/13	0.26	0.76	64,65,66,66	11
10	TRD	D	7	13/13	0.17	0.70	41,43,50,50	0
10	TRD	B	1023	9/13	0.12	0.67	58,59,60,61	0
7	OH	A	1501	1/1	0.23	0.57	35,35,35,35	0
5	MG	A	1006	1/1	0.20	0.46	16,16,16,16	0
9	HEA	A	1502	60/60	0.19	0.38	23,26,33,34	0
7	OH	C	572	1/1	0.23	0.33	28,28,28,28	0
9	HEA	C	574	60/60	0.18	0.29	23,26,32,33	0
9	HEA	A	1503	60/60	0.18	0.22	26,29,41,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	HEA	C	575	60/60	0.21	0.19	21,24,32,33	0
10	TRD	C	577	13/13	0.14	0.07	45,50,53,54	0
3	DMU	B	1011	23/33	0.16	-0.72	57,58,58,58	23
4	CU	D	4	1/1	0.10	-0.89	28,28,28,28	0
6	CA	A	1007	1/1	0.08	-0.97	27,27,27,27	0
4	CU	C	569	1/1	0.12	-1.44	26,26,26,26	0
11	CD	D	9	1/1	0.05	-1.47	46,46,46,46	0
4	CU	B	1022	1/1	0.10	-1.49	28,28,28,28	0
11	CD	B	1010	1/1	0.08	-1.62	53,53,53,53	1
4	CU	D	3	1/1	0.09	-1.64	28,28,28,28	0
6	CA	C	571	1/1	0.06	-1.64	32,32,32,32	0
4	CU	B	1004	1/1	0.09	-1.72	29,29,29,29	0
11	CD	D	8	1/1	0.05	-2.08	36,36,36,36	0
11	CD	B	1008	1/1	0.06	-2.56	35,35,35,35	0
11	CD	B	1009	1/1	0.05	-2.74	45,45,45,45	1
4	CU	A	1023	1/1	0.12	-3.24	32,32,32,32	0
3	DMU	A	1002	22/33	0.21	-	66,66,67,67	22

6.5 Other polymers ⓘ

There are no such residues in this entry.