



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:47 PM GMT

PDB ID : 1QLE
Title : CRYO-STRUCTURE OF THE PARACOCCLUS DENITRIFICANS FOUR-SUBUNIT CYTOCHROME C OXIDASE IN THE COMPLETELY OXIDIZED STATE COMPLEXED WITH AN ANTIBODY FV FRAGMENT
Authors : Harrenga, A.; Michel, H.
Deposited on : 1999-08-30
Resolution : 3.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

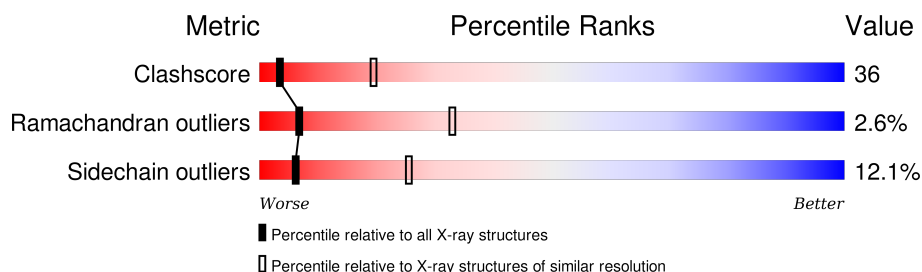
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	538	 35% 56% 8%
2	B	252	 46% 46% 8%
3	C	273	 45% 48% 8%
4	D	43	 63% 33% 5%
5	H	119	 31% 64% 5%
6	L	108	 41% 50% 9%

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
8	HEA	X	1	X	-	-	-
8	HEA	X	2	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10762 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 POLYPEPTIDE I-BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4269	2860	671	705	33			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			1977	1295	319	355	8			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	273	Total	C	N	O	S	0	0	0
			2181	1483	339	348	11			

- Molecule 4 is a protein called CCYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	43	Total	C	N	O	S	0	0	0
			332	214	58	59	1			

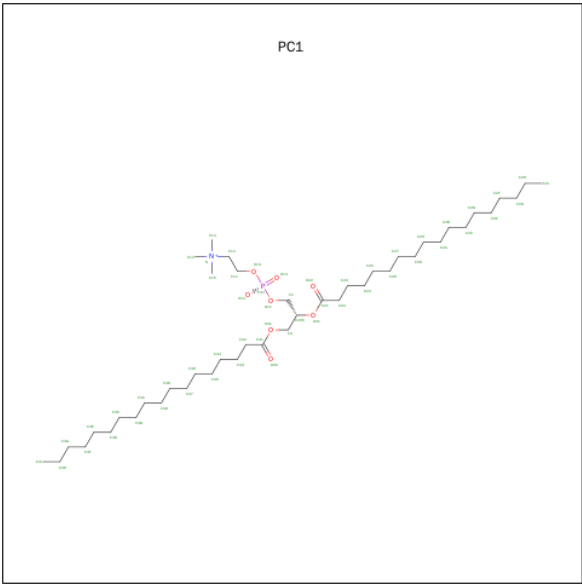
- Molecule 5 is a protein called HEAVY CHAIN ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	119	Total	C	N	O	S	0	0	0
			938	589	157	186	6			

- Molecule 6 is a protein called LIGHT CHAIN ANTIBODY FV FRAGMENT.

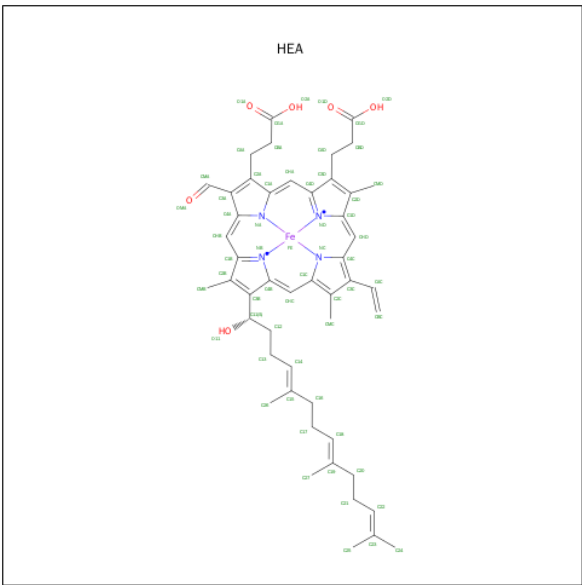
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	108	Total	C	N	O	S	0	0	0
			832	530	135	165	2			

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



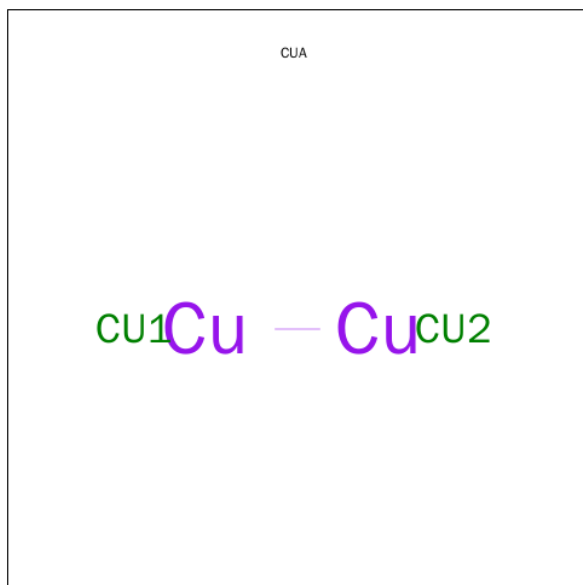
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	P	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
7	P	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	Y	1	Total	Cu	0	0
			2	2		

- Molecule 10 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	Y	1	Total	Cu	0	0
			1	1		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	Z	1	Total	Ca	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

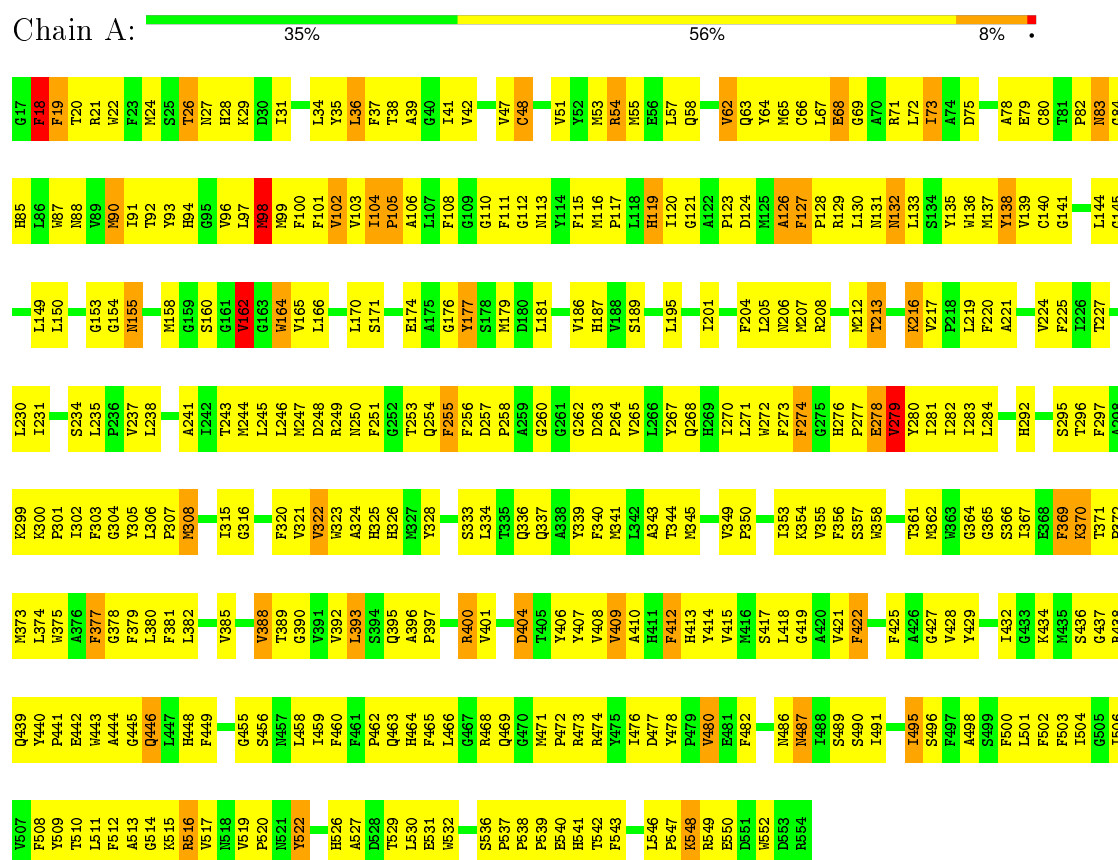
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	Z	1	Total 1	Mn 1	0	0

3 Residue-property plots

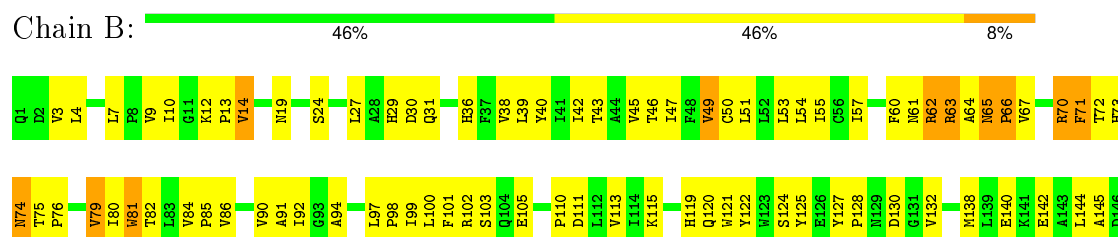
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

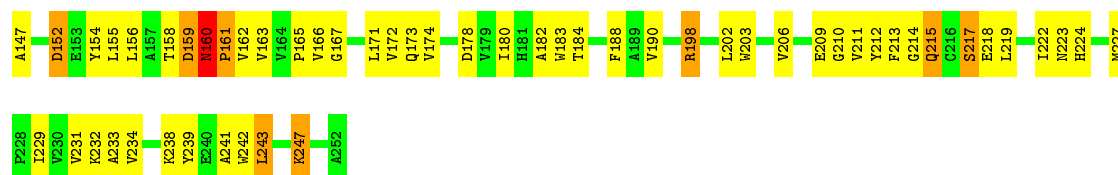
Note EDS was not executed.

• Molecule 1: CYTOCHROME C OXIDASE POLYPEPTIDE I-BETA

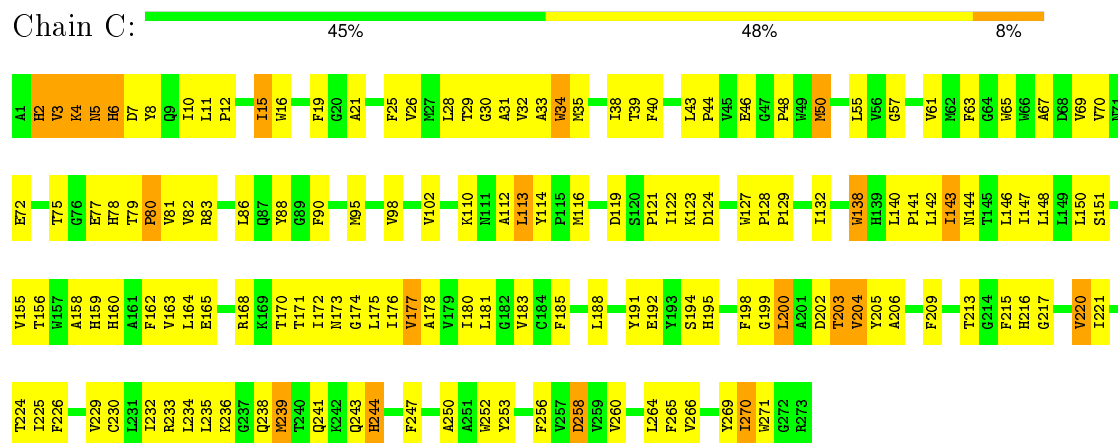


• Molecule 2: CYTOCHROME C OXIDASE POLYPEPTIDE II

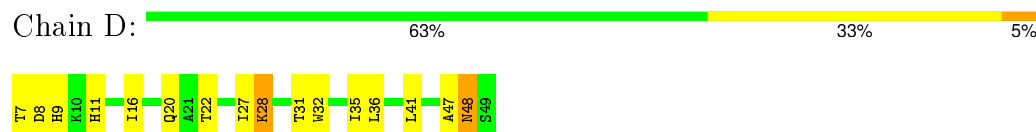




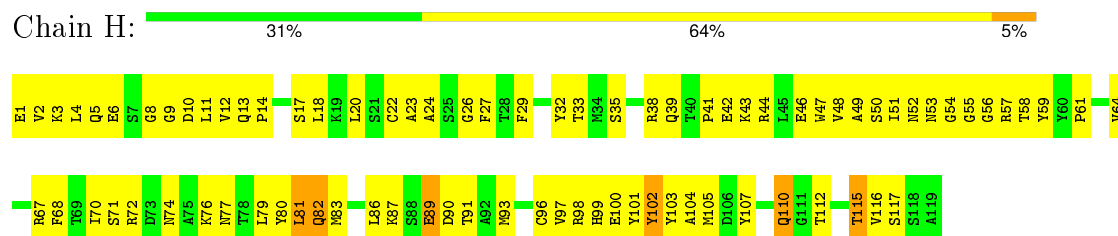
• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE III



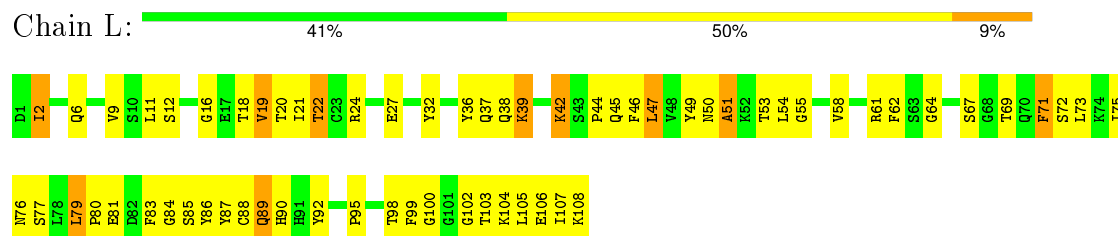
• Molecule 4: CCYTOCHROME C OXIDASE



• Molecule 5: HEAVY CHAIN ANTIBODY FV FRAGMENT



• Molecule 6: LIGHT CHAIN ANTIBODY FV FRAGMENT



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	205.20 Å 205.20 Å 81.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	66.2 (6.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.235 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10762	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: PC1, CA, MN, HEA, CUA, CU

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	0.59	0/4428	0.74	3/6042 (0.0%)
2	B	0.56	0/2034	0.75	0/2787
3	C	0.56	1/2267 (0.0%)	0.70	1/3103 (0.0%)
4	D	0.49	0/339	0.66	1/457 (0.2%)
5	H	0.59	0/960	0.73	0/1298
6	L	0.53	0/853	0.74	0/1156
All	All	0.57	1/10881 (0.0%)	0.73	5/14843 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	252	TRP	CB-CG	6.38	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ARG	NE-CZ-NH2	7.20	123.90	120.30
3	C	35	MET	CG-SD-CE	6.13	110.01	100.20
1	A	98	MET	CG-SD-CE	6.00	109.80	100.20
1	A	99	MET	CG-SD-CE	5.90	109.65	100.20
4	D	36	LEU	CA-CB-CG	5.12	127.07	115.30

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	4269	0	4184	366	0
2	B	1977	0	1963	148	0
3	C	2181	0	2151	178	0
4	D	332	0	331	12	0
5	H	938	0	894	72	0
6	L	832	0	807	54	0
7	P	108	0	176	26	0
8	X	120	0	108	32	0
9	Y	2	0	0	0	0
10	Y	1	0	0	0	0
11	Z	1	0	0	0	0
12	Z	1	0	0	0	0
All	All	10762	0	10614	778	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 36.

The worst 5 of 778 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:B:4:LEU:HD11	2:B:242:TRP:CD1	1.25	1.68
2:B:4:LEU:CD1	2:B:242:TRP:CD1	2.15	1.27
3:C:2:HIS:O	3:C:3:VAL:HG22	1.13	1.25
5:H:6:GLU:OE1	5:H:96:CYS:N	1.66	1.25
2:B:159:ASP:O	2:B:161:PRO:HD3	1.37	1.22

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	536/538 (100%)	447 (83%)	71 (13%)	18 (3%)	5	25
2	B	250/252 (99%)	198 (79%)	47 (19%)	5 (2%)	9	41
3	C	271/273 (99%)	215 (79%)	51 (19%)	5 (2%)	11	45
4	D	41/43 (95%)	33 (80%)	5 (12%)	3 (7%)	1	6
5	H	117/119 (98%)	99 (85%)	16 (14%)	2 (2%)	11	46
6	L	106/108 (98%)	92 (87%)	13 (12%)	1 (1%)	21	64
All	All	1321/1333 (99%)	1084 (82%)	203 (15%)	34 (3%)	7	33

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	213	THR
1	A	442	GLU
1	A	19	PHE
1	A	102	VAL

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	441/441 (100%)	387 (88%)	54 (12%)	6	25
2	B	211/211 (100%)	183 (87%)	28 (13%)	5	21
3	C	220/220 (100%)	197 (90%)	23 (10%)	8	32
4	D	34/34 (100%)	28 (82%)	6 (18%)	2	12
5	H	101/101 (100%)	91 (90%)	10 (10%)	10	35
6	L	92/92 (100%)	80 (87%)	12 (13%)	5	22
All	All	1099/1099 (100%)	966 (88%)	133 (12%)	6	25

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	65	ASN

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Mol	Chain	Res	Type
2	B	161	PRO
6	L	19	VAL
2	B	70	ARG
2	B	111	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	521	ASN
2	B	36	HIS
5	H	39	GLN
1	A	541	HIS
2	B	65	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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
7	PC1	P	2	-	53,53,53	1.46	2 (3%)	57,61,61	1.03	2 (3%)
7	PC1	P	3	-	53,53,53	1.36	3 (5%)	57,61,61	0.93	3 (5%)
8	HEA	X	1	1	40,67,67	1.46	6 (15%)	41,103,103	1.22	4 (9%)
8	HEA	X	2	1	40,67,67	1.73	9 (22%)	41,103,103	1.15	5 (12%)
9	CUA	Y	1	2	0,1,1	0.00	-	0,0,0	0.00	-

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
7	PC1	P	2	-	-	2/57/57/57	0/0/0/0
7	PC1	P	3	-	-	0/57/57/57	0/0/0/0
8	HEA	X	1	1	3/3/7/16	0/24/76/76	0/0/8/8
8	HEA	X	2	1	3/3/7/16	0/24/76/76	0/0/8/8
9	CUA	Y	1	2	-	0/0/0/0	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	2	HEA	C3C-CAC	-4.66	1.37	1.47
8	X	1	HEA	C3A-C2A	-4.13	1.34	1.40
8	X	2	HEA	C3C-C2C	-4.13	1.34	1.40
8	X	1	HEA	C3C-CAC	-3.52	1.40	1.47
8	X	2	HEA	C3A-C2A	-3.22	1.36	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	2	PC1	C3-C2-C1	-4.89	100.64	112.07
8	X	1	HEA	C17-C18-C19	-3.33	120.53	127.76
7	P	3	PC1	C11-C12-N	-2.91	106.68	116.03
7	P	3	PC1	C3-O31-C31	-2.83	108.93	116.85
8	X	1	HEA	C13-C14-C15	-2.78	121.71	127.76

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	X	1	HEA	ND

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Mol	Chain	Res	Type	Atom
8	X	1	HEA	NA
8	X	1	HEA	NB
8	X	2	HEA	ND
8	X	2	HEA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	2	PC1	C2-O21-C21-O22
7	P	2	PC1	C2-O21-C21-C22

There are no ring outliers.

4 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	2	PC1	10	0
7	P	3	PC1	16	0
8	X	1	HEA	20	0
8	X	2	HEA	12	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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.