wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:22 AM GMT

PDB ID	:	2GSM
Title	:	Catalytic Core (Subunits I and II) of Cytochrome c oxidase from Rhodobacter sphaeroides
Authors	:	Qin, L.; Hiser, C.; Mulichak, A.; Garavito, R.M.; Ferguson-Miller, S.
Deposited on	:	2006-04-26
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

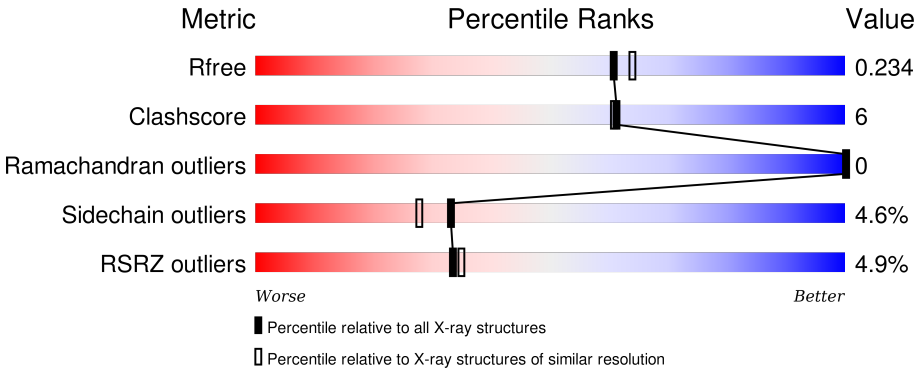
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	566	3% 82% 11% • 5%
1	C	566	8% 81% 12% • 6%
2	B	262	2% 85% 11% ••
2	D	262	3% 85% 11% ••

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	TRD	A	5009	-	-	-	X
10	TRD	A	5010	-	-	-	X
10	TRD	B	5008	-	-	-	X
10	TRD	C	6009	-	-	-	X
10	TRD	C	6010	-	-	-	X
10	TRD	D	6007	-	-	-	X
10	TRD	D	6008	-	-	-	X
3	DMU	A	5002	-	-	-	X
3	DMU	B	5003	-	-	-	X
3	DMU	C	6005	-	-	-	X
5	MG	A	3006	-	-	-	X
9	HEA	A	2001	X	-	-	-
9	HEA	A	2002	X	-	-	-
9	HEA	C	3001	X	-	-	-
9	HEA	C	3002	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13644 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 subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	26	0	0
			4212	2822	663	696	31			
1	C	534	Total	C	N	O	S	44	0	0
			4201	2813	662	695	31			

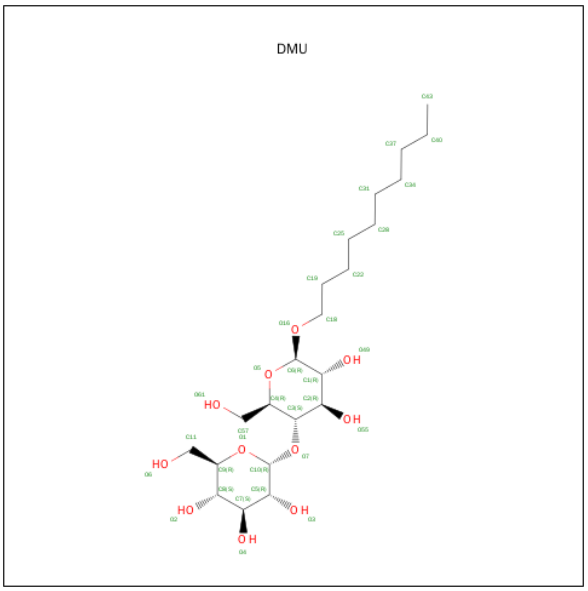
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	9	0	0
			2025	1321	333	365	6			
2	D	256	Total	C	N	O	S	13	0	0
			2025	1321	333	365	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: $C_{22}H_{42}O_{11}$).



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

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

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

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

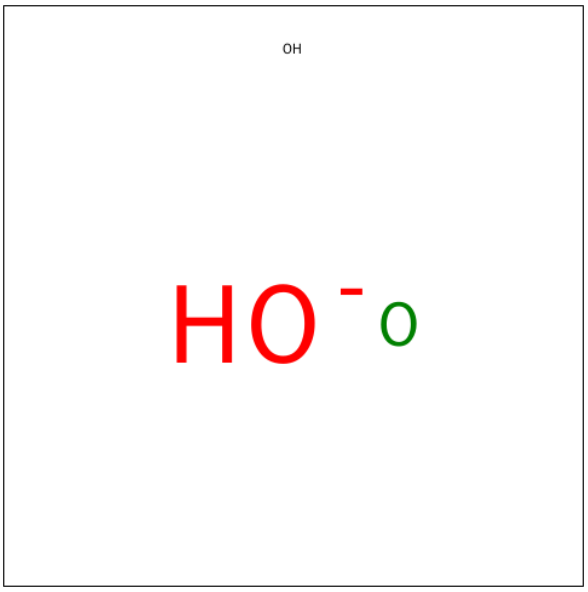
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

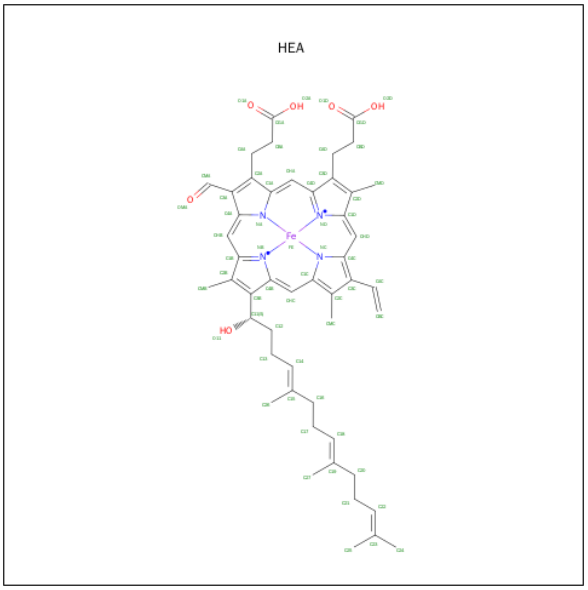
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Cd 2 2	0	0
7	D	2	Total Cd 2 2	0	0

- Molecule 8 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 9 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

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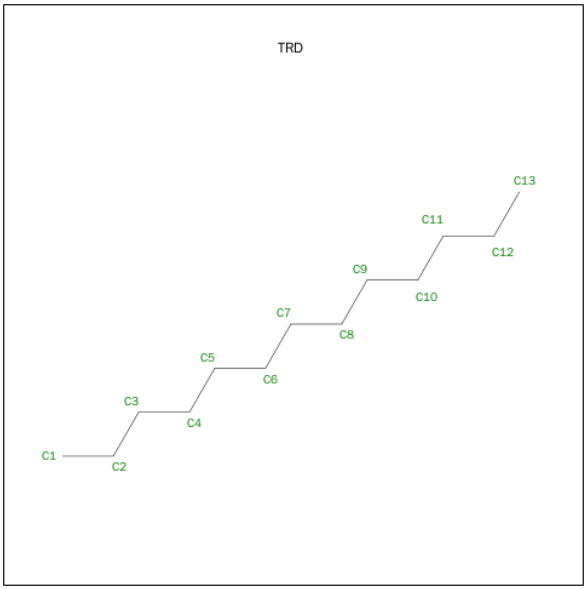
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C Fe N O 60 49 1 4 6	0	0
9	C	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 10 is TRIDECANE (three-letter code: TRD) (formula: $C_{13}H_{28}$).



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

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

- Molecule 11 is water.

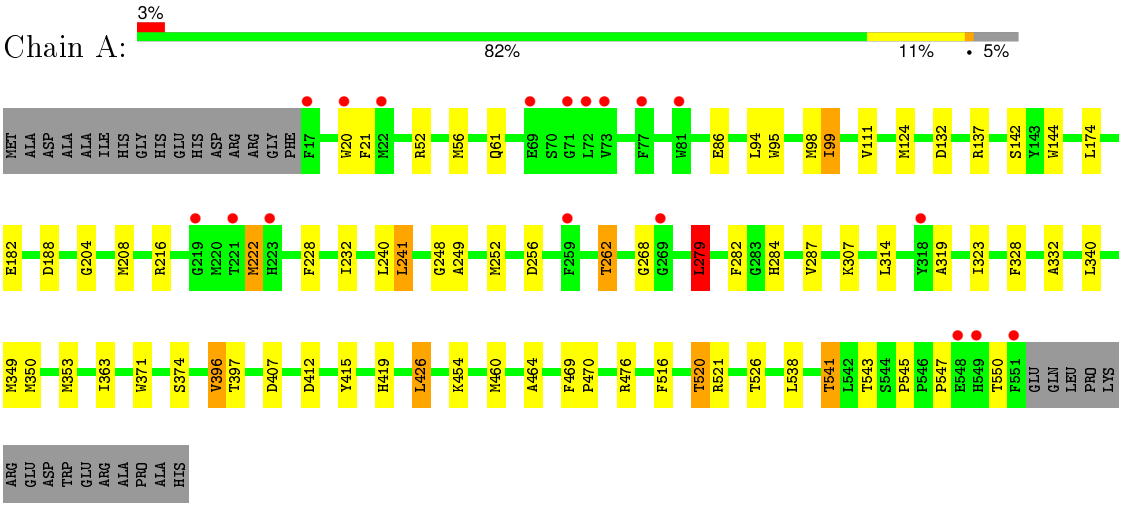
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	140	Total O 140 140	0	0
11	B	142	Total O 142 142	0	0
11	C	100	Total O 100 100	0	0
11	D	121	Total O 121 121	0	0

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.

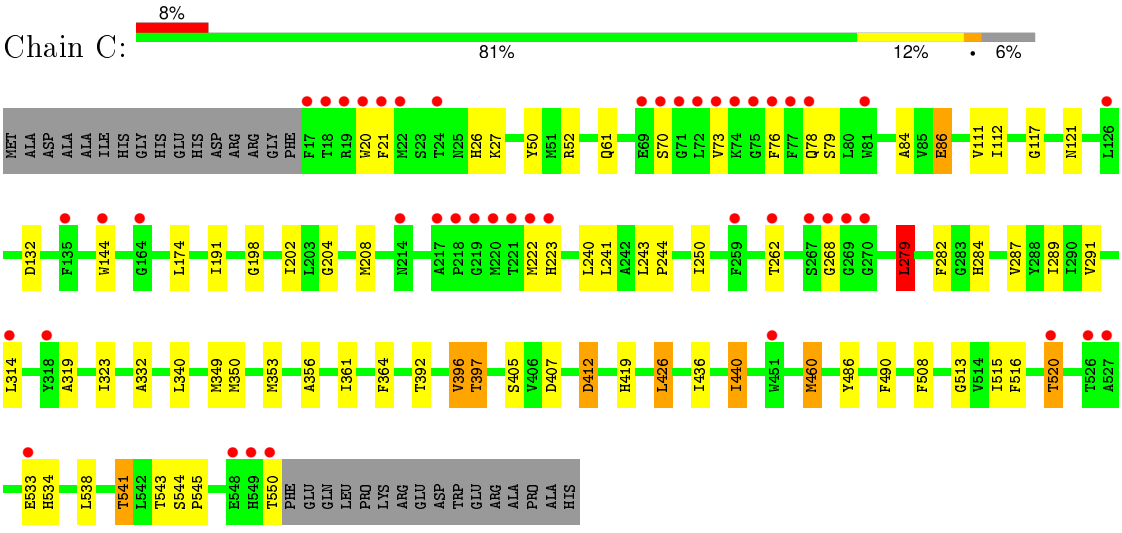
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



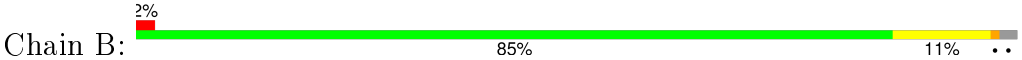
- Molecule 1: Cytochrome c oxidase subunit 1

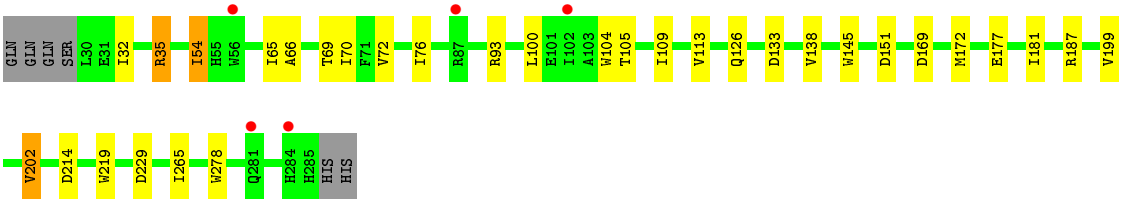
Chain C:



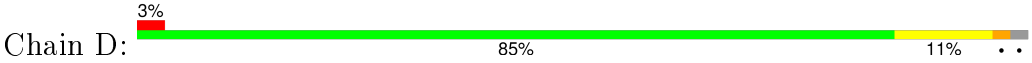
- Molecule 2: Cytochrome c oxidase subunit 2

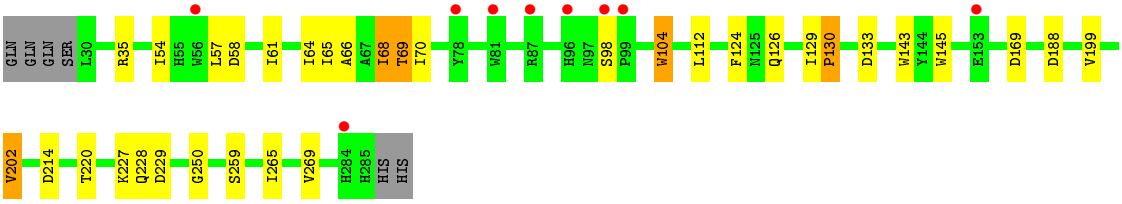
Chain B:





- Molecule 2: Cytochrome c oxidase subunit 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.02Å 131.64Å 176.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.00) 96.1 (19.91-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.214 , 0.232 0.215 , 0.234	Depositor DCC
R_{free} test set	3780 reflections (2.05%)	DCC
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.7	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 188619 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13644	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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, CA, TRD, CD, DMU, 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	0/4368	0.67	6/5961 (0.1%)
1	C	0.51	0/4356	0.63	5/5945 (0.1%)
2	B	0.53	0/2087	0.72	8/2857 (0.3%)
2	D	0.51	0/2087	0.69	5/2857 (0.2%)
All	All	0.54	0/12898	0.67	24/17620 (0.1%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	229	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	407	ASP	CB-CG-OD2	6.63	124.27	118.30
2	D	169	ASP	CB-CG-OD2	6.37	124.03	118.30
2	B	214	ASP	CB-CG-OD2	6.26	123.93	118.30
2	B	133	ASP	CB-CG-OD2	6.15	123.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4212	0	4134	53	0
1	C	4201	0	4125	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2025	0	1982	20	0
2	D	2025	0	1982	19	0
3	A	99	0	126	0	0
3	B	56	0	63	3	0
3	C	89	0	105	2	0
3	D	46	0	42	2	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	B	2	0	0	0	0
7	D	2	0	0	0	0
8	A	1	0	0	1	0
8	C	1	0	0	1	0
9	A	120	0	108	7	0
9	C	120	0	108	4	0
10	A	59	0	125	4	0
10	B	9	0	17	2	0
10	C	44	0	90	2	0
10	D	20	0	41	0	0
11	A	140	0	0	3	0
11	B	142	0	0	1	0
11	C	100	0	0	2	0
11	D	121	0	0	1	0
All	All	13644	0	13048	143	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 6.

The worst 5 of 143 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:228:PHE:CE2	1:A:232:ILE:HD11	1.96	1.00
1:A:350:MET:HA	1:A:353:MET:HE3	1.51	0.91
1:C:397:THR:HG22	1:C:419:HIS:HB2	1.54	0.90
8:A:6501:OH:O	11:A:6506:HOH:O	1.95	0.83
1:A:460:MET:CE	1:A:464:ALA:HB2	2.08	0.83

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	533/566 (94%)	520 (98%)	13 (2%)	0	100	100
1	C	532/566 (94%)	519 (98%)	13 (2%)	0	100	100
2	B	254/262 (97%)	248 (98%)	6 (2%)	0	100	100
2	D	254/262 (97%)	247 (97%)	7 (3%)	0	100	100
All	All	1573/1656 (95%)	1534 (98%)	39 (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	435/459 (95%)	413 (95%)	22 (5%)	29	23
1	C	434/459 (95%)	410 (94%)	24 (6%)	27	21
2	B	215/221 (97%)	211 (98%)	4 (2%)	65	67
2	D	215/221 (97%)	205 (95%)	10 (5%)	32	27
All	All	1299/1360 (96%)	1239 (95%)	60 (5%)	33	28

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	ARG
1	C	174	LEU
2	D	130	PRO
1	C	78	GLN
1	C	240	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	251	GLN
1	C	26	HIS
2	D	88	ASN
2	B	228	GLN
1	C	223	HIS

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 42 ligands modelled in this entry, 2 are modelled with single atom and 14 are monoatomic - leaving 26 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	$\#\|Z\|>2$
9	HEA	A	2001	1	40,67,67	1.66	6 (15%)	41,103,103	1.52	8 (19%)
9	HEA	A	2002	1,11	40,67,67	1.35	4 (10%)	41,103,103	1.68	10 (24%)
3	DMU	A	5001	-	34,34,34	0.49	0	45,45,45	1.02	2 (4%)
3	DMU	A	5002	-	34,34,34	0.55	0	45,45,45	0.99	4 (8%)
3	DMU	A	5004	-	34,34,34	0.51	0	45,45,45	1.02	4 (8%)
10	TRD	A	5005	-	12,12,12	0.28	0	11,11,11	0.58	0
10	TRD	A	5006	-	12,12,12	0.28	0	11,11,11	0.54	0
10	TRD	A	5007	-	12,12,12	0.22	0	11,11,11	0.52	0
10	TRD	A	5009	-	6,6,12	0.31	0	5,5,11	0.38	0
10	TRD	A	5010	-	12,12,12	0.27	0	11,11,11	0.56	0
3	DMU	B	5003	-	34,34,34	0.52	0	45,45,45	0.68	0
10	TRD	B	5008	-	8,8,12	0.26	0	7,7,11	0.48	0
3	DMU	B	5011	-	24,24,34	0.59	0	35,35,45	1.22	4 (11%)
9	HEA	C	3001	1	40,67,67	1.66	6 (15%)	41,103,103	1.43	6 (14%)
9	HEA	C	3002	1,11	40,67,67	1.42	3 (7%)	41,103,103	1.55	8 (19%)
10	TRD	C	6001	-	12,12,12	0.30	0	11,11,11	0.52	0
3	DMU	C	6002	-	24,24,34	0.58	0	35,35,45	0.72	0
3	DMU	C	6004	-	34,34,34	0.65	1 (2%)	45,45,45	0.89	2 (4%)
3	DMU	C	6005	-	34,34,34	0.68	1 (2%)	45,45,45	1.49	11 (24%)
10	TRD	C	6006	-	12,12,12	0.27	0	11,11,11	0.62	0
10	TRD	C	6009	-	8,8,12	0.29	0	7,7,11	0.48	0
10	TRD	C	6010	-	8,8,12	0.30	0	7,7,11	0.47	0
3	DMU	D	6003	-	24,24,34	0.57	0	35,35,45	0.78	1 (2%)
10	TRD	D	6007	-	12,12,12	0.24	0	11,11,11	0.61	0
10	TRD	D	6008	-	6,6,12	0.25	0	5,5,11	0.40	0
3	DMU	D	6011	-	24,24,34	0.56	0	35,35,45	1.30	6 (17%)

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
9	HEA	A	2001	1	3/3/7/16	0/24/76/76	0/0/8/8
9	HEA	A	2002	1,11	3/3/7/16	0/24/76/76	0/0/8/8
3	DMU	A	5001	-	-	0/19/59/59	0/2/2/2
3	DMU	A	5002	-	-	0/19/59/59	0/2/2/2
3	DMU	A	5004	-	-	0/19/59/59	0/2/2/2
10	TRD	A	5005	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	TRD	A	5006	-	-	0/10/10/10	0/0/0/0
10	TRD	A	5007	-	-	0/10/10/10	0/0/0/0
10	TRD	A	5009	-	-	0/4/4/10	0/0/0/0
10	TRD	A	5010	-	-	0/10/10/10	0/0/0/0
3	DMU	B	5003	-	-	0/19/59/59	0/2/2/2
10	TRD	B	5008	-	-	0/6/6/10	0/0/0/0
3	DMU	B	5011	-	-	0/8/48/59	0/2/2/2
9	HEA	C	3001	1	2/2/7/16	0/24/76/76	0/0/8/8
9	HEA	C	3002	1,11	3/3/7/16	0/24/76/76	0/0/8/8
10	TRD	C	6001	-	-	0/10/10/10	0/0/0/0
3	DMU	C	6002	-	-	0/8/48/59	0/2/2/2
3	DMU	C	6004	-	-	0/19/59/59	0/2/2/2
3	DMU	C	6005	-	-	0/19/59/59	0/2/2/2
10	TRD	C	6006	-	-	0/10/10/10	0/0/0/0
10	TRD	C	6009	-	-	0/6/6/10	0/0/0/0
10	TRD	C	6010	-	-	0/6/6/10	0/0/0/0
3	DMU	D	6003	-	-	0/8/48/59	0/2/2/2
10	TRD	D	6007	-	-	0/10/10/10	0/0/0/0
10	TRD	D	6008	-	-	0/4/4/10	0/0/0/0
3	DMU	D	6011	-	-	0/8/48/59	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2001	HEA	C3A-C2A	-6.34	1.32	1.40
9	C	3001	HEA	C3A-C2A	-6.02	1.32	1.40
9	C	3002	HEA	C3A-C2A	-4.43	1.34	1.40
9	C	3001	HEA	C3C-C2C	-4.29	1.34	1.40
9	A	2001	HEA	C3C-C2C	-4.08	1.34	1.40

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2002	HEA	CAD-CBD-CGD	-5.17	103.27	112.75
9	A	2001	HEA	C4B-C3B-C11	-3.94	122.72	127.01
3	C	6005	DMU	C10-O7-C3	-3.84	107.96	118.01
9	C	3002	HEA	CAD-CBD-CGD	-3.71	105.94	112.75
9	A	2002	HEA	CAD-C3D-C4D	-3.39	123.33	127.01

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	2002	HEA	ND
9	A	2002	HEA	NA
9	A	2002	HEA	NB
9	A	2001	HEA	ND
9	A	2001	HEA	NA

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2001	HEA	1	0
9	A	2002	HEA	6	0
10	A	5005	TRD	2	0
10	A	5006	TRD	2	0
10	A	5007	TRD	2	0
3	B	5003	DMU	3	0
10	B	5008	TRD	2	0
9	C	3001	HEA	2	0
9	C	3002	HEA	2	0
10	C	6001	TRD	1	0
3	C	6004	DMU	1	0
3	C	6005	DMU	1	0
10	C	6006	TRD	1	0
3	D	6003	DMU	1	0
3	D	6011	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

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, 95^{th} 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	535/566 (94%)	-0.08	18 (3%) 49 50	19, 30, 47, 58	6 (1%)
1	C	534/566 (94%)	0.25	46 (8%) 13 14	25, 41, 54, 60	9 (1%)
2	B	256/262 (97%)	-0.14	5 (1%) 68 69	21, 33, 44, 50	2 (0%)
2	D	256/262 (97%)	0.05	9 (3%) 48 49	26, 37, 50, 55	3 (1%)
All	All	1581/1656 (95%)	0.04	78 (4%) 33 35	19, 35, 51, 60	20 (1%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	PHE	7.8
1	C	20	TRP	6.6
1	C	18	THR	6.3
1	C	81	TRP	6.1
1	C	222	MET	5.7

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, 95^{th} 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(Å^2)	Q<0.9
10	TRD	C	6009	9/13	0.81	0.32	13.05	48,49,53,53	0
10	TRD	A	5010	13/13	0.78	0.28	10.78	46,49,56,56	0
3	DMU	A	5002	33/33	0.88	0.24	7.47	48,51,55,57	0
3	DMU	C	6005	33/33	0.71	0.27	7.32	44,53,57,57	33
10	TRD	A	5009	7/13	0.76	0.21	4.35	48,51,52,52	0
5	MG	A	3006	1/1	0.99	0.18	3.75	10,10,10,10	0
10	TRD	C	6010	9/13	0.91	0.20	3.38	50,51,52,52	0
10	TRD	D	6008	7/13	0.91	0.19	3.38	44,44,45,45	0
10	TRD	B	5008	9/13	0.92	0.20	3.29	44,45,46,46	0
10	TRD	D	6007	13/13	0.88	0.16	2.45	45,46,49,49	0
3	DMU	B	5003	33/33	0.88	0.23	2.32	48,52,58,58	0
3	DMU	C	6004	33/33	0.82	0.28	1.61	46,59,100,100	11
5	MG	C	4006	1/1	0.99	0.14	1.44	12,12,12,12	0
10	TRD	C	6001	13/13	0.82	0.20	1.37	49,50,53,53	0
10	TRD	A	5005	13/13	0.92	0.12	1.23	39,41,48,48	0
10	TRD	A	5007	13/13	0.94	0.12	0.66	35,38,40,42	0
3	DMU	A	5004	33/33	0.82	0.17	0.52	35,54,100,100	11
3	DMU	A	5001	33/33	0.94	0.11	0.35	24,33,44,44	0
9	HEA	A	2001	60/60	0.98	0.10	0.10	17,21,26,27	0
4	CU	B	3004	1/1	1.00	0.10	-0.14	24,24,24,24	0
9	HEA	C	3001	60/60	0.98	0.10	-0.41	26,29,40,41	0
9	HEA	A	2002	60/60	0.98	0.09	-0.43	21,25,32,35	0
4	CU	D	4004	1/1	1.00	0.09	-0.65	29,29,29,29	0
6	CA	A	3007	1/1	0.99	0.09	-0.89	24,24,24,24	0
9	HEA	C	3002	60/60	0.98	0.08	-0.98	26,30,38,39	0
4	CU	B	3003	1/1	1.00	0.07	-1.12	24,24,24,24	0
6	CA	C	4007	1/1	0.98	0.06	-1.94	34,34,34,34	0
4	CU	D	4003	1/1	1.00	0.08	-1.95	27,27,27,27	0
7	CD	B	3008	1/1	0.99	0.05	-2.12	35,35,35,35	0
7	CD	D	4008	1/1	0.99	0.05	-2.51	35,35,35,35	0
7	CD	B	3009	1/1	0.99	0.04	-4.70	40,40,40,40	1
8	OH	C	7501	1/1	0.97	0.09	-	35,35,35,35	0
3	DMU	D	6003	23/33	0.84	0.23	-	50,52,55,56	23
3	DMU	C	6002	23/33	0.81	0.35	-	56,57,57,58	23
3	DMU	D	6011	23/33	0.71	0.28	-	53,55,57,57	23
3	DMU	B	5011	23/33	0.63	0.24	-	51,54,57,59	23
8	OH	A	6501	1/1	0.97	0.12	-	26,26,26,26	0
10	TRD	C	6006	13/13	0.90	0.34	-	51,52,53,54	0
7	CD	D	4009	1/1	0.99	0.02	-	42,42,42,42	1
10	TRD	A	5006	13/13	0.90	0.30	-	49,51,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CU	C	4005	1/1	0.99	0.04	-	33,33,33,33	0
4	CU	A	3005	1/1	0.99	0.06	-	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.