



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:31 am GMT

PDB ID : 1M57
Title : Structure of cytochrome c oxidase from Rhodobacter sphaeroides (EQ(I-286 mutant))
Authors : Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.
Deposited on : 2002-07-08
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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

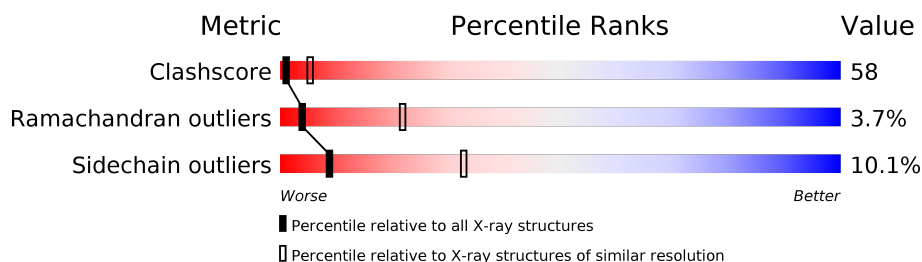
1 Overall quality at a glance

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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (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	566	
1	G	566	
2	B	264	
2	H	264	
3	C	266	
3	I	266	
4	D	51	

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Mol	Chain	Length	Quality of chain
4	J	51	

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	A	1001	X	-	-	-
8	HEA	A	1002	X	-	-	-
8	HEA	G	1001	X	-	X	-
8	HEA	G	1002	X	-	-	-
9	PEH	C	2010	-	-	X	-
9	PEH	C	2013	-	-	X	-
9	PEH	G	3012	-	-	X	-
9	PEH	I	3010	-	-	X	-
9	PEH	I	3013	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18934 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4322	2892	685	714	31			
1	G	547	Total	C	N	O	S	0	0	0
			4322	2892	685	714	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	GLN	GLU	ENGINEERED	UNP P33517
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	286	GLN	GLU	ENGINEERED	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			
2	H	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			
3	I	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			
4	J	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Cu	0	0
			2	2		
5	G	1	Total	Cu	0	0
			1	1		
5	B	2	Total	Cu	0	0
			2	2		
5	A	1	Total	Cu	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mg	0	0
			1	1		

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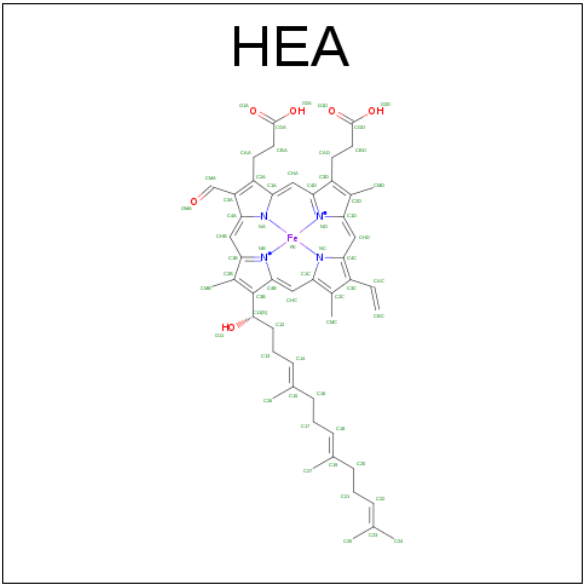
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

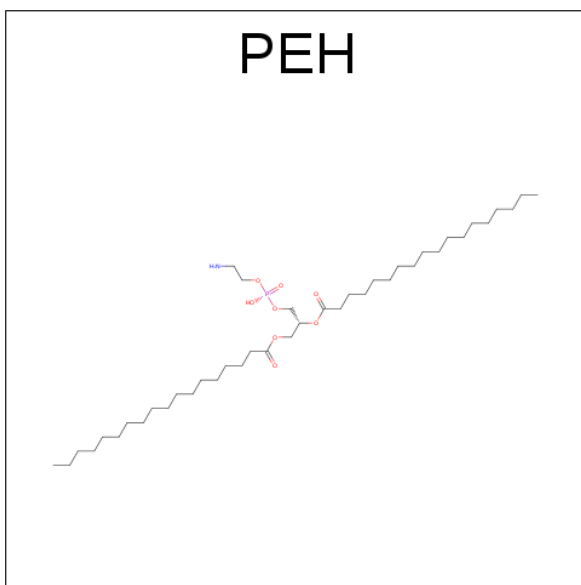
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 9 is DI-STEAROYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEH) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	J	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	97	Total 97	O 97	0	0
10	B	70	Total 70	O 70	0	0
10	C	38	Total 38	O 38	0	0
10	D	13	Total 13	O 13	0	0
10	G	107	Total 107	O 107	0	0
10	H	64	Total 64	O 64	0	0
10	I	37	Total 37	O 37	0	0
10	J	10	Total 10	O 10	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 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.

Note EDS was not executed.

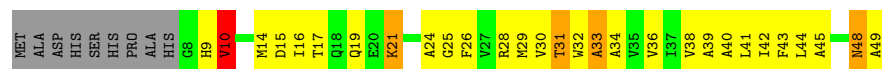
• Molecule 1: CYTOCHROME C OXIDASE





- Molecule 2: CYTOCHROME C OXIDASE

S168	S169	S170	S171	S172	S173	S174	S175	S176	S177	S178	S179	S180	S181	S182	S183	S184	S185	S186	S187	S188	S189	S190	S191	S192	S193	S194	S195	S196	S197	S198	S199	S200	S201	S202	S203	S204	S205	S206	S207	S208	S209	S210	S211	S212	S213	S214	S215	S216	S217	S218	S219	S220	S221	S222
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4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	340.72 Å 340.72 Å 89.76 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	4.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (4.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.293 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEH, CA, 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	0.73	0/4482	2.01	128/6114 (2.1%)
1	G	0.75	1/4482 (0.0%)	2.06	133/6114 (2.2%)
2	B	0.60	0/2105	1.93	56/2879 (1.9%)
2	H	0.65	0/2105	1.96	58/2879 (2.0%)
3	C	0.57	0/2232	1.66	33/3054 (1.1%)
3	I	0.59	0/2232	1.65	30/3054 (1.0%)
4	D	0.58	0/316	1.63	4/428 (0.9%)
4	J	0.60	0/316	1.63	4/428 (0.9%)
All	All	0.67	1/18270 (0.0%)	1.91	446/24950 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	G	0	16
2	B	0	6
2	H	0	3
3	C	0	5
3	I	0	7
4	D	0	1
All	All	0	57

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	112	ILE	N-CA	5.08	1.56	1.46

The worst 5 of 446 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	52	ARG	NE-CZ-NH2	-24.46	108.07	120.30
2	B	171	ARG	NE-CZ-NH1	19.39	130.00	120.30
1	A	543	THR	C-N-CA	19.24	169.80	121.70
1	G	543	THR	C-N-CA	16.53	163.02	121.70
2	H	171	ARG	NE-CZ-NH1	15.75	128.17	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	114	ALA	Mainchain
1	A	29	ILE	Mainchain
1	A	96	ASN	Mainchain

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	4322	0	4240	609	0
1	G	4322	0	4240	621	0
2	B	2046	0	2011	219	0
2	H	2046	0	2011	231	0
3	C	2139	0	2056	224	0
3	I	2139	0	2056	214	0
4	D	311	0	319	33	0
4	J	311	0	319	40	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	120	0	108	40	0
8	G	120	0	108	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	102	0	162	38	0
9	C	153	0	243	56	0
9	D	51	0	81	17	0
9	G	102	0	162	41	0
9	I	153	0	243	59	0
9	J	51	0	81	13	0
10	A	97	0	0	26	0
10	B	70	0	0	20	0
10	C	38	0	0	8	0
10	D	13	0	0	0	0
10	G	107	0	0	30	0
10	H	64	0	0	18	0
10	I	37	0	0	7	0
10	J	10	0	0	1	0
All	All	18934	0	18440	2141	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 58.

The worst 5 of 2141 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:G:379:THR:HB	1:G:380:PRO:HD3	1.18	1.17
1:A:106:MET:HG2	8:A:1001:HEA:HAC	1.17	1.16
9:C:2010:PEH:H3I2	9:C:2010:PEH:H3E2	1.22	1.13
9:I:3010:PEH:C3I	9:I:3010:PEH:H3E2	1.78	1.13
8:A:1002:HEA:HMC1	8:A:1002:HEA:HBC1	1.30	1.11

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	545/566 (96%)	416 (76%)	106 (19%)	23 (4%)	3	18
1	G	545/566 (96%)	403 (74%)	112 (21%)	30 (6%)	2	12
2	B	258/264 (98%)	203 (79%)	47 (18%)	8 (3%)	5	26
2	H	258/264 (98%)	206 (80%)	44 (17%)	8 (3%)	5	26
3	C	263/266 (99%)	217 (82%)	41 (16%)	5 (2%)	9	41
3	I	263/266 (99%)	209 (80%)	49 (19%)	5 (2%)	9	41
4	D	40/51 (78%)	26 (65%)	13 (32%)	1 (2%)	6	32
4	J	40/51 (78%)	26 (65%)	12 (30%)	2 (5%)	2	15
All	All	2212/2294 (96%)	1706 (77%)	424 (19%)	82 (4%)	4	22

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	160	PRO
1	A	544	SER
1	A	545	PRO
2	B	254	GLU

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	446/459 (97%)	397 (89%)	49 (11%)	7	28
1	G	446/459 (97%)	397 (89%)	49 (11%)	7	28
2	B	216/220 (98%)	195 (90%)	21 (10%)	9	35
2	H	216/220 (98%)	196 (91%)	20 (9%)	10	38
3	C	215/216 (100%)	198 (92%)	17 (8%)	14	46
3	I	215/216 (100%)	195 (91%)	20 (9%)	10	38
4	D	30/37 (81%)	25 (83%)	5 (17%)	2	13
4	J	30/37 (81%)	27 (90%)	3 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1814/1864 (97%)	1630 (90%)	184 (10%)	9 33

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	166	TRP
1	G	147	VAL
3	I	95	SER
3	C	204	MET
1	G	52	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	231	HIS
1	G	165	GLN
3	I	212	HIS
1	G	26	HIS
1	G	286	GLN

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 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	HEA	A	1001	1	44,67,67	1.72	6 (13%)	37,103,103	2.48	21 (56%)
8	HEA	A	1002	1	44,67,67	1.79	7 (15%)	37,103,103	2.11	9 (24%)
9	PEH	A	2009	-	50,50,50	1.58	3 (6%)	52,55,55	1.13	3 (5%)
9	PEH	A	2012	-	50,50,50	1.58	3 (6%)	52,55,55	1.44	6 (11%)
9	PEH	C	2008	-	50,50,50	1.55	2 (4%)	52,55,55	1.22	6 (11%)
9	PEH	C	2010	-	50,50,50	1.50	2 (4%)	52,55,55	1.13	3 (5%)
9	PEH	C	2013	-	50,50,50	1.55	3 (6%)	52,55,55	1.34	3 (5%)
9	PEH	D	2011	-	50,50,50	1.46	3 (6%)	52,55,55	1.31	7 (13%)
8	HEA	G	1001	1	44,67,67	1.79	7 (15%)	37,103,103	2.54	19 (51%)
8	HEA	G	1002	1	44,67,67	1.51	6 (13%)	37,103,103	2.01	13 (35%)
9	PEH	G	3009	-	50,50,50	1.46	3 (6%)	52,55,55	1.00	2 (3%)
9	PEH	G	3012	-	50,50,50	1.59	2 (4%)	52,55,55	1.28	6 (11%)
9	PEH	I	3008	-	50,50,50	1.61	2 (4%)	52,55,55	1.17	3 (5%)
9	PEH	I	3010	-	50,50,50	1.57	4 (8%)	52,55,55	1.02	2 (3%)
9	PEH	I	3013	-	50,50,50	1.60	3 (6%)	52,55,55	1.22	3 (5%)
9	PEH	J	3011	-	50,50,50	1.66	2 (4%)	52,55,55	1.54	7 (13%)

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	HEA	A	1001	1	3/3/7/16	0/24/76/76	0/0/8/8
8	HEA	A	1002	1	3/3/7/16	0/24/76/76	0/0/8/8
9	PEH	A	2009	-	-	0/54/54/54	0/0/0/0
9	PEH	A	2012	-	-	0/54/54/54	0/0/0/0
9	PEH	C	2008	-	-	0/54/54/54	0/0/0/0
9	PEH	C	2010	-	-	0/54/54/54	0/0/0/0
9	PEH	C	2013	-	-	0/54/54/54	0/0/0/0
9	PEH	D	2011	-	-	0/54/54/54	0/0/0/0
8	HEA	G	1001	1	3/3/7/16	0/24/76/76	0/0/8/8
8	HEA	G	1002	1	3/3/7/16	0/24/76/76	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEH	G	3009	-	-	0/54/54/54	0/0/0/0
9	PEH	G	3012	-	-	0/54/54/54	0/0/0/0
9	PEH	I	3008	-	-	0/54/54/54	0/0/0/0
9	PEH	I	3010	-	-	0/54/54/54	0/0/0/0
9	PEH	I	3013	-	-	0/54/54/54	0/0/0/0
9	PEH	J	3011	-	-	0/54/54/54	0/0/0/0

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1002	HEA	C3A-C2A	-6.14	1.32	1.40
8	A	1002	HEA	C3C-C2C	-5.73	1.32	1.40
8	A	1001	HEA	C3C-C2C	-5.34	1.33	1.40
8	G	1001	HEA	C3C-C2C	-5.29	1.33	1.40
8	G	1001	HEA	C3C-CAC	-4.89	1.38	1.47

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	2013	PEH	C2-O21-C21	-6.75	101.93	117.88
9	J	3011	PEH	C2-O21-C21	-6.53	102.44	117.88
8	A	1002	HEA	C13-C14-C15	-5.94	112.75	127.68
9	I	3013	PEH	C2-O21-C21	-5.69	104.44	117.88
8	G	1002	HEA	C13-C14-C15	-5.27	114.44	127.68

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1001	HEA	ND
8	A	1001	HEA	NA
8	A	1001	HEA	NB
8	G	1001	HEA	ND
8	G	1001	HEA	NA

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 283 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1001	HEA	20	0
8	A	1002	HEA	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2009	PEH	18	0
9	A	2012	PEH	20	0
9	C	2008	PEH	13	0
9	C	2010	PEH	24	0
9	C	2013	PEH	21	0
9	D	2011	PEH	17	0
8	G	1001	HEA	23	0
8	G	1002	HEA	15	0
9	G	3009	PEH	19	0
9	G	3012	PEH	22	0
9	I	3008	PEH	13	0
9	I	3010	PEH	24	0
9	I	3013	PEH	22	0
9	J	3011	PEH	13	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.