



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:17 AM GMT

PDB ID : 3OMN  
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with D132A mutation in the reduced state  
Authors : Liu, J.; Qin, L.; Ferguson-Miller, S.  
Deposited on : 2010-08-27  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

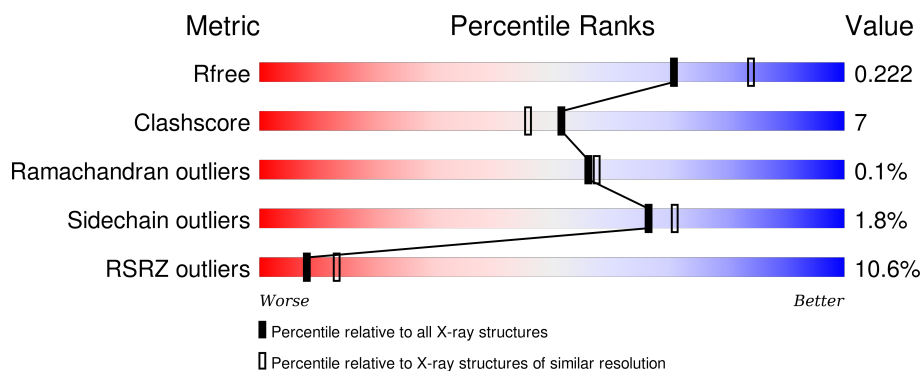
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div>7%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	535	<div> <div>20%</div> <div>85%</div> <div>14%</div> <div>..</div> </div>
2	B	256	<div> <div>3%</div> <div>95%</div> <div>.</div> </div>
2	D	256	<div> <div>5%</div> <div>93%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

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

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13755 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase, aa3 type, subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	13	0
			4274	2862	673	707	32			
1	C	531	Total	C	N	O	S	0	13	0
			4219	2826	663	698	32			

There are 2 discrepancies between the modelled and reference sequences:

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

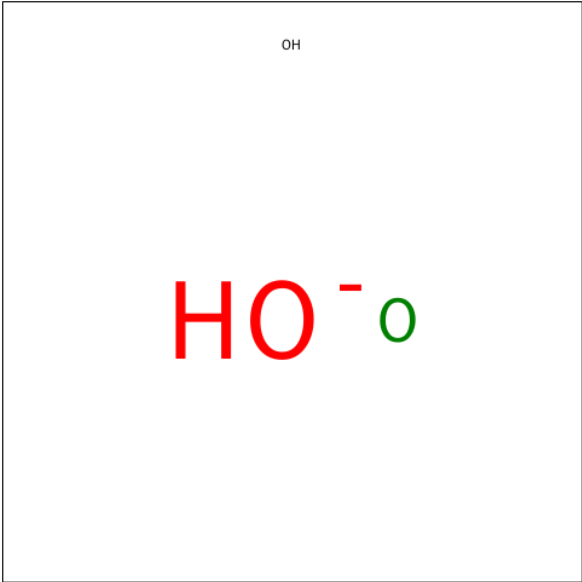
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

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

There are 8 discrepancies between the modelled and reference sequences:

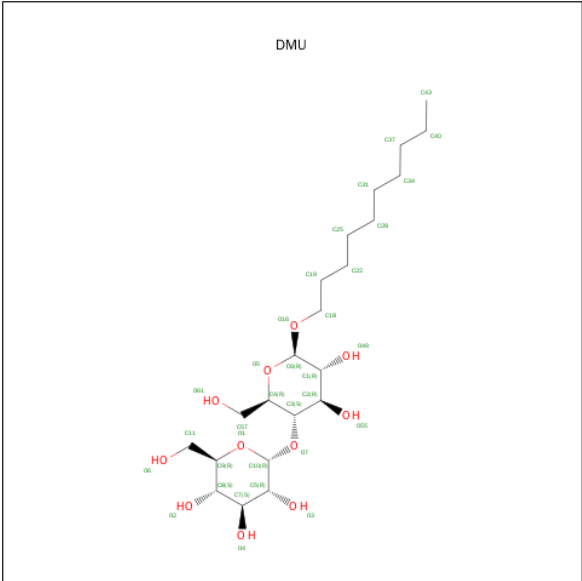
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	284	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	285	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	284	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	285	HIS	-	EXPRESSION TAG	UNP Q3J5G0

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 4 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



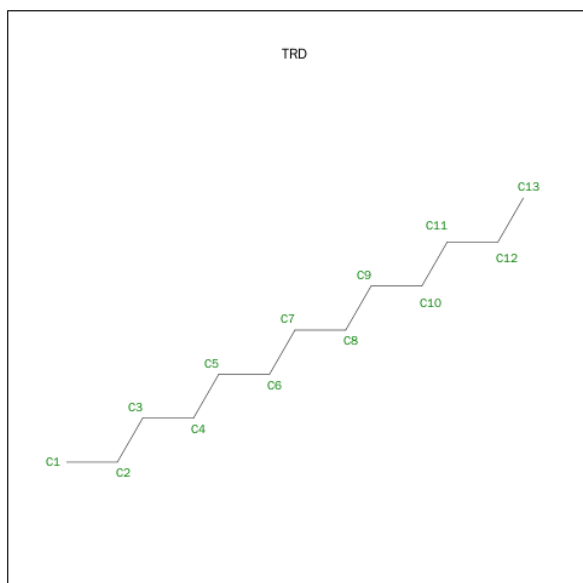
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 16 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	16	5		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			33	22	11		
4	D	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is TRIDECANE (three-letter code: TRD) (formula:  $C_{13}H_{28}$ ).



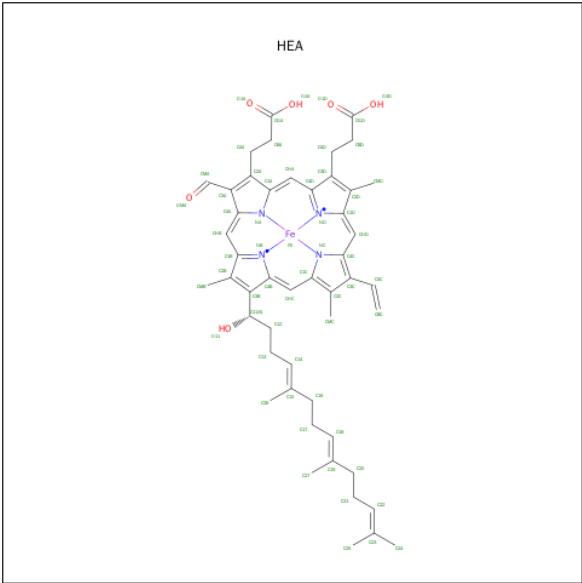
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			7	7		

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

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



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

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

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

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

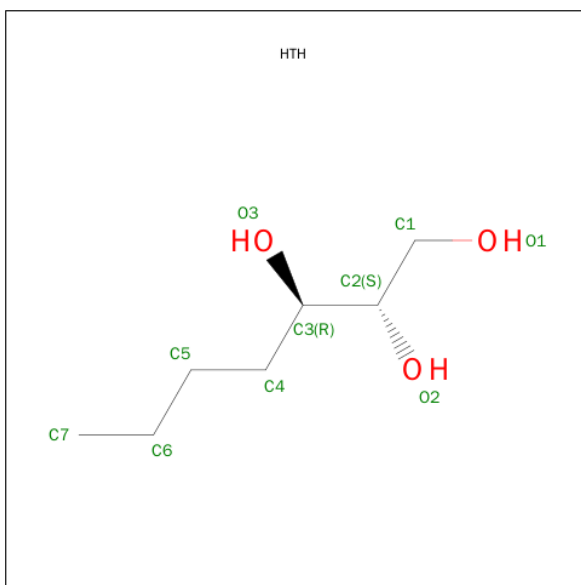
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		

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

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

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





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

- Molecule 12 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

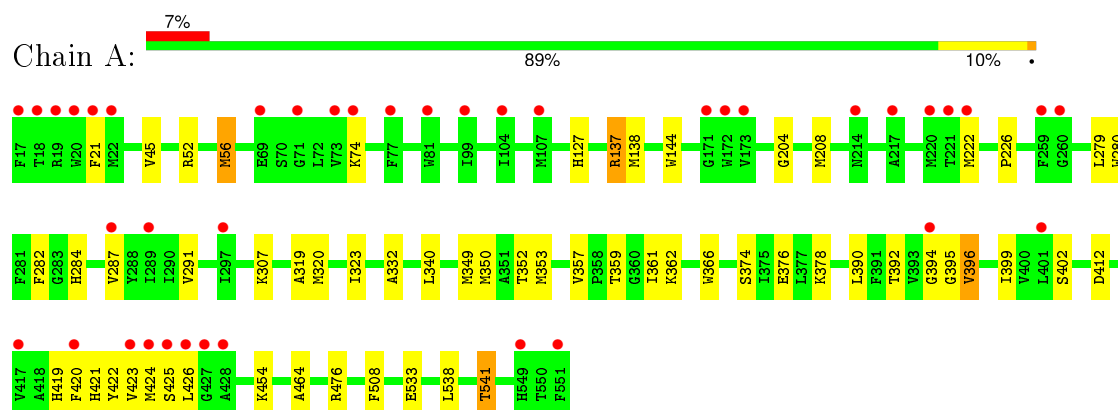
- Molecule 13 is water.

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

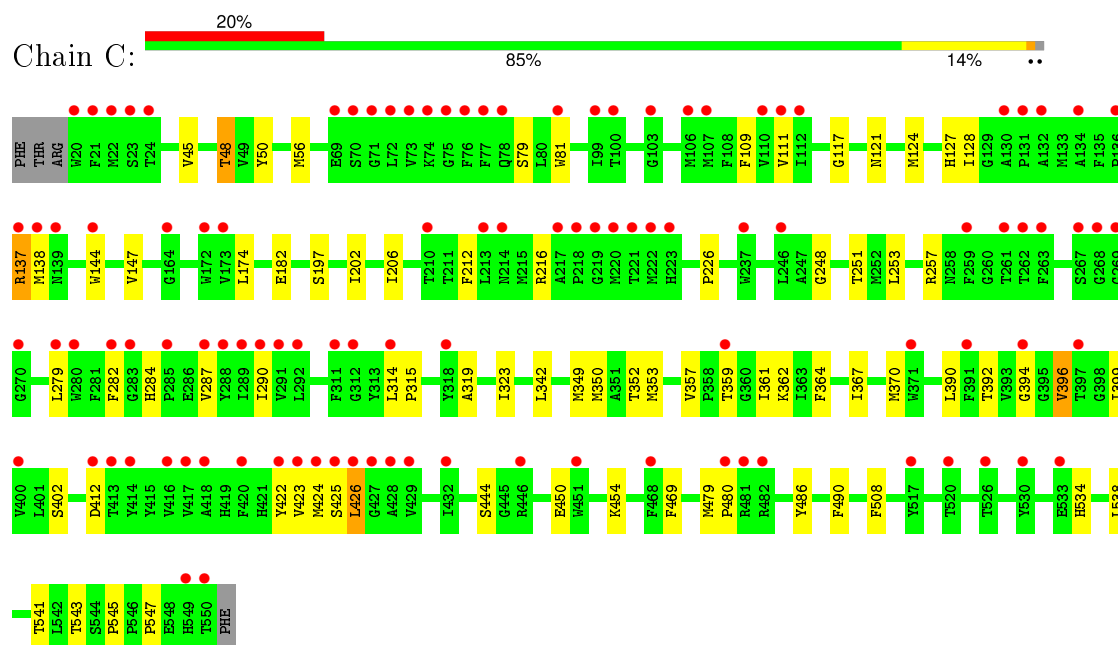
### 3 Residue-property plots

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, aa3 type, subunit I

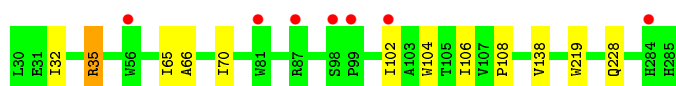


- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

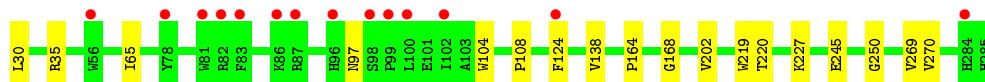
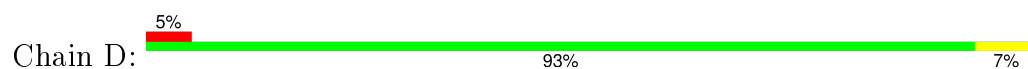


- Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 2: Cytochrome c oxidase subunit 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.67Å 132.03Å 176.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 2.15 42.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.70-2.15) 97.2 (42.70-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.198 , 0.219 0.200 , 0.222	Depositor DCC
$R_{free}$ test set	4627 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 74.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 153587 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

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

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CU1, OH, CA, CL, TRD, CD, DMU, HTH, HEA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.54	0/4430	0.55	0/6048
1	C	0.46	0/4373	0.53	0/5973
2	B	0.50	0/2083	0.56	0/2852
2	D	0.46	0/2077	0.52	0/2845
All	All	0.49	0/12963	0.54	0/17718

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4274	0	4182	68	0
1	C	4219	0	4120	87	0
2	B	2021	0	1978	10	0
2	D	2015	0	1967	14	0
3	A	1	0	0	1	0
3	C	1	0	0	1	0
4	A	43	0	61	2	0
4	B	122	0	147	0	0
4	C	79	0	84	2	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.03	1.17
1:A:357:VAL:O	1:A:361[B]:ILE:HG12	1.52	1.07
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:HG	1.41	1.00
1:C:422[A]:TYR:CD2	1:C:426[A]:LEU:HD12	1.97	0.99
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.30	0.93
1:A:390:LEU:HD13	1:A:426[A]:LEU:HB3	1.50	0.92
1:C:390:LEU:HD13	1:C:426[A]:LEU:HB3	1.52	0.91
1:A:137:ARG:NH1	1:A:137:ARG:HG3	1.83	0.91
6:C:1:HEA:HBC1	6:C:1:HEA:HMC1	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH11	1:A:137:ARG:CG	1.85	0.90
3:A:802:OH:O	13:A:701[A]:HOH:O	1.90	0.89
1:C:357:VAL:O	1:C:361[B]:ILE:HG12	1.74	0.88
6:C:2[B]:HEA:HMD1	6:C:2[B]:HEA:HBD2	1.57	0.84
1:C:422[A]:TYR:CE2	1:C:426[A]:LEU:HD12	2.11	0.84
3:C:802:OH:O	13:C:701:HOH:O	1.96	0.84
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.41	0.83
6:A:1:HEA:HBC1	6:A:1:HEA:HMC1	1.59	0.83
2:B:228:GLN:NE2	13:B:777:HOH:O	2.12	0.82
1:C:137:ARG:HH11	1:C:137:ARG:CG	1.95	0.80
1:A:426[A]:LEU:CD2	1:A:464:ALA:HB1	2.13	0.78
1:C:422[A]:TYR:O	1:C:426[A]:LEU:HB2	1.82	0.78
1:A:137:ARG:HD2	1:A:138:MET:H	1.47	0.78
1:C:48:THR:HG23	6:C:1:HEA:HMB3	1.68	0.76
6:A:2[B]:HEA:HBD2	6:A:2[B]:HEA:HMD1	1.68	0.75
1:C:56:MET:HE1	4:C:10:DMU:H6	1.69	0.74
2:B:66:ALA:O	2:B:70:ILE:HG12	1.86	0.74
1:C:48:THR:HG21	6:C:1:HEA:O11	1.86	0.74
1:A:425[A]:SER:C	1:A:426[A]:LEU:HD23	2.09	0.73
1:C:182:GLU:O	1:C:257:ARG:NH1	2.22	0.73
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:CG	2.20	0.72
1:A:399:ILE:HD13	6:A:2[B]:HEA:HMB1	1.72	0.72
1:A:422[A]:TYR:CD2	1:A:426[A]:LEU:HD12	2.26	0.71
2:B:32:ILE:HG22	2:B:35:ARG:HD3	1.72	0.70
1:C:287:VAL:HB	6:C:2[B]:HEA:HAC	1.75	0.69
1:A:426[A]:LEU:HD21	1:A:464:ALA:HB1	1.76	0.68
1:A:287:VAL:HB	6:A:2[B]:HEA:HAC	1.75	0.67
1:C:144:TRP:CE3	1:C:147:VAL:HG11	2.30	0.67
1:C:534:HIS:HD2	13:C:629:HOH:O	1.78	0.66
1:A:426[A]:LEU:HD22	1:A:464:ALA:HB1	1.78	0.66
1:A:402:SER:HA	6:A:2[B]:HEA:OMA	1.96	0.65
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.30	0.65
1:A:396:VAL:HG13	2:B:65:ILE:HB	1.78	0.63
1:A:320:MET:HG3	1:A:362[B]:LYS:HE3	1.81	0.63
1:C:137:ARG:NH1	1:C:137:ARG:HG3	2.09	0.63
1:C:137:ARG:HD2	1:C:138:MET:H	1.64	0.62
2:D:202:VAL:HG23	2:D:270:VAL:O	2.01	0.61
1:C:359[A]:THR:HG21	6:C:2[A]:HEA:C14	2.30	0.61
1:C:144:TRP:HE3	1:C:147:VAL:HG11	1.66	0.61
1:C:424[A]:MET:HG2	6:C:2[A]:HEA:CBC	2.30	0.61
1:C:396:VAL:HG13	2:D:65:ILE:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422[A]:TYR:HA	1:A:426[A]:LEU:HG	1.83	0.60
1:C:425[A]:SER:C	1:C:426[A]:LEU:HD23	2.22	0.60
1:C:248:GLY:O	1:C:251:THR:HG22	2.01	0.60
1:A:137:ARG:HD2	1:A:138:MET:N	2.15	0.60
1:A:424[A]:MET:HG2	6:A:2[A]:HEA:CBC	2.31	0.60
4:D:8:DMU:H35	4:D:8:DMU:H29	1.82	0.59
1:C:424[A]:MET:HG2	6:C:2[A]:HEA:HBC2	1.84	0.59
1:C:319:ALA:HB3	1:C:362[B]:LYS:HE2	1.85	0.58
2:D:202:VAL:CG2	2:D:245:GLU:HG2	2.33	0.58
1:C:394:GLY:HA3	1:C:423[A]:VAL:HG13	1.86	0.58
1:A:352:THR:HG22	6:A:2[B]:HEA:HMB2	1.87	0.57
1:A:361[B]:ILE:HD11	2:B:108:PRO:HG2	1.86	0.57
1:C:137:ARG:NH1	1:C:137:ARG:CG	2.64	0.56
1:A:425[A]:SER:O	1:A:426[A]:LEU:HD23	2.05	0.56
1:C:392:THR:HG23	6:C:2[B]:HEA:H171	1.87	0.56
1:C:284:HIS:O	1:C:287:VAL:HG22	2.03	0.56
1:C:253:LEU:O	1:C:257:ARG:HG3	2.06	0.56
1:C:399:ILE:HD13	6:C:2[B]:HEA:HMB1	1.88	0.55
1:A:422[A]:TYR:CE2	1:A:426[A]:LEU:HD12	2.42	0.55
1:A:424[A]:MET:HG2	6:A:2[A]:HEA:HBC2	1.89	0.55
1:C:543:THR:HG23	1:C:545:PRO:O	2.07	0.55
1:A:538:LEU:O	1:A:541:THR:HB	2.06	0.55
1:C:50:TYR:OH	1:C:79:SER:HB2	2.06	0.54
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:HB2	1.88	0.54
1:A:307:LYS:HE2	1:A:374:SER:HB3	1.90	0.53
1:C:399:ILE:HG13	6:C:2[A]:HEA:H242	1.89	0.53
1:C:111:VAL:HG11	1:C:290:ILE:HG23	1.89	0.53
1:A:396:VAL:CG1	2:B:65:ILE:HB	2.38	0.53
1:C:394:GLY:C	1:C:423[B]:VAL:HG13	2.29	0.53
1:A:454:LYS:HE3	13:A:758:HOH:O	2.07	0.53
1:C:394:GLY:CA	1:C:422[B]:TYR:HB3	2.39	0.52
1:C:396:VAL:CG1	2:D:65:ILE:HB	2.39	0.52
1:A:399:ILE:HD13	6:A:2[B]:HEA:CMB	2.37	0.52
1:C:124:MET:CE	1:C:212:PHE:HD2	2.22	0.52
1:C:352:THR:HG22	6:C:2[B]:HEA:HMB2	1.91	0.52
2:B:35:ARG:HD2	13:B:743:HOH:O	2.10	0.52
1:A:419[B]:HIS:CE1	1:A:423[B]:VAL:HG21	2.45	0.52
6:C:2[B]:HEA:CBD	6:C:2[B]:HEA:HMD1	2.36	0.51
1:A:350:MET:HA	1:A:353:MET:CE	2.39	0.51
1:A:392:THR:HG23	6:A:2[B]:HEA:H171	1.93	0.51
1:C:361[B]:ILE:HD11	2:D:108:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:HA	1:A:353:MET:HE2	1.93	0.51
1:C:422[A]:TYR:CA	1:C:426[A]:LEU:HB2	2.41	0.50
1:C:48:THR:HG23	6:C:1:HEA:CMB	2.38	0.50
1:C:127:HIS:HB3	1:C:226:PRO:HG2	1.94	0.50
1:C:444:SER:HA	4:C:9:DMU:H5	1.94	0.50
1:C:284:HIS:CD2	1:C:284:HIS:C	2.85	0.50
1:A:476:ARG:HH21	5:A:3:TRD:H31	1.77	0.49
1:A:399:ILE:HG13	6:A:2[A]:HEA:H242	1.93	0.49
1:C:350:MET:HA	1:C:353:MET:CE	2.42	0.49
1:A:394:GLY:HA3	1:A:423[A]:VAL:HG13	1.94	0.49
1:C:402:SER:HA	6:C:2[B]:HEA:OMA	2.12	0.49
1:A:359[A]:THR:HG21	6:A:2[A]:HEA:H14	1.93	0.49
1:A:56:MET:HE1	4:A:1005:DMU:H6	1.93	0.49
1:C:367:ILE:HA	1:C:370:MET:CE	2.42	0.49
1:A:137:ARG:NH1	1:A:137:ARG:CG	2.55	0.49
1:A:45:VAL:HG21	6:A:1:HEA:H171	1.95	0.49
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:CB	2.43	0.49
1:A:284:HIS:CD2	1:A:284:HIS:C	2.87	0.48
1:C:202:ILE:O	1:C:206:ILE:HG12	2.13	0.48
2:D:202:VAL:HG21	2:D:245:GLU:HG2	1.93	0.48
1:C:538:LEU:O	1:C:541:THR:HB	2.14	0.48
1:A:395:GLY:O	6:A:2[B]:HEA:H121	2.12	0.48
2:B:102:ILE:O	2:B:106:ILE:HG12	2.13	0.47
1:C:508:PHE:HB2	6:C:1:HEA:H261	1.97	0.47
2:D:30:LEU:N	13:D:728:HOH:O	2.47	0.47
1:C:128:ILE:HB	1:C:216:ARG:HB3	1.95	0.47
1:C:543:THR:HG22	1:C:547:PRO:HD3	1.97	0.47
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.96	0.47
1:C:45:VAL:HG21	6:C:1:HEA:H171	1.96	0.47
1:A:508:PHE:HB2	6:A:1:HEA:H261	1.97	0.47
1:A:332:ALA:HB1	1:A:340:LEU:HD11	1.97	0.46
1:C:359[A]:THR:HG22	6:C:2[A]:HEA:H172	1.98	0.46
1:C:117:GLY:O	1:C:121:ASN:HB2	2.15	0.46
1:A:533:GLU:H	1:A:533:GLU:CD	2.19	0.46
1:C:361[B]:ILE:O	1:C:364:PHE:N	2.46	0.46
1:C:367:ILE:HA	1:C:370:MET:HE2	1.98	0.46
1:A:204:GLY:O	1:A:208:MET:HG2	2.16	0.46
1:C:396:VAL:HG13	2:D:65:ILE:HD12	1.98	0.46
1:C:144:TRP:O	1:C:147:VAL:HG12	2.17	0.45
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.51	0.45
1:A:395:GLY:N	1:A:423[B]:VAL:HG13	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ALA:HB3	1:A:362[B]:LYS:HE2	1.97	0.45
4:A:1005:DMU:H8	5:A:553:TRD:H71	1.99	0.45
1:C:422[A]:TYR:O	1:C:426[A]:LEU:CB	2.61	0.44
1:A:396:VAL:HG13	2:B:65:ILE:HD12	1.98	0.44
1:C:349:MET:HG2	1:C:353:MET:HE2	2.00	0.44
1:C:342:LEU:HD21	2:D:124:PHE:CD2	2.52	0.44
1:A:426[A]:LEU:HD22	1:A:464:ALA:CB	2.47	0.44
1:A:287:VAL:HB	6:A:2[A]:HEA:CAC	2.47	0.44
1:C:422[A]:TYR:OH	1:C:469:PHE:HB2	2.19	0.43
1:C:81:TRP:CZ2	5:C:552:TRD:H92	2.54	0.43
2:D:202:VAL:HG21	2:D:245:GLU:CG	2.48	0.43
1:C:314:LEU:HB3	1:C:315:PRO:HD3	2.00	0.43
6:A:2[B]:HEA:H212	6:A:2[B]:HEA:H18	1.78	0.43
1:A:362[A]:LYS:HD3	1:A:366:TRP:CH2	2.54	0.43
1:A:280:TRP:CH2	6:A:2[A]:HEA:HBD1	2.54	0.43
1:A:279:LEU:C	1:A:279:LEU:HD13	2.39	0.43
1:C:422[A]:TYR:C	1:C:426[A]:LEU:HB2	2.39	0.43
1:A:420:PHE:HA	1:A:423[A]:VAL:HG22	2.00	0.43
1:C:349:MET:O	1:C:353:MET:HG3	2.18	0.43
1:A:349:MET:O	1:A:353:MET:HG3	2.19	0.43
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.54	0.43
1:A:280:TRP:HH2	6:A:2[A]:HEA:HBD1	1.83	0.42
1:A:320:MET:CG	1:A:362[B]:LYS:HE3	2.49	0.42
1:A:394:GLY:CA	1:A:422[B]:TYR:HB3	2.50	0.42
1:C:392:THR:O	1:C:396:VAL:HB	2.19	0.42
1:C:350:MET:HA	1:C:353:MET:HE3	2.02	0.42
1:A:376:GLU:HG2	1:A:378:LYS:HG2	2.02	0.42
1:C:399:ILE:HD13	6:C:2[B]:HEA:CMB	2.50	0.42
2:D:202:VAL:HG22	2:D:269:VAL:HG12	2.02	0.42
2:D:164:PRO:HA	2:D:168:GLY:O	2.20	0.42
1:A:426[A]:LEU:HD23	1:A:426[A]:LEU:N	2.35	0.42
1:C:323:ILE:HD11	1:C:359[B]:THR:HA	2.02	0.42
1:C:450:GLU:HG3	1:C:454:LYS:HE2	2.02	0.42
2:D:220:THR:O	2:D:250:GLY:HA3	2.20	0.42
1:C:422[A]:TYR:O	1:C:426[A]:LEU:C	2.58	0.42
1:C:144:TRP:HA	1:C:147:VAL:HG12	2.01	0.42
1:C:399:ILE:HG13	6:C:2[A]:HEA:C24	2.50	0.41
1:C:424[A]:MET:CE	6:C:2[A]:HEA:HMD3	2.50	0.41
1:A:421:HIS:HA	1:A:425[B]:SER:HB2	2.02	0.41
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.55	0.41
1:A:323:ILE:HD11	1:A:359[B]:THR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422[A]:TYR:O	1:A:426[A]:LEU:HB2	2.21	0.41
1:A:350:MET:HG2	1:A:353:MET:CE	2.51	0.41
1:C:350:MET:HG2	1:C:353:MET:CE	2.50	0.41
1:C:479:MET:HA	1:C:480:PRO:HD3	1.95	0.41
1:C:486:TYR:CD2	1:C:490:PHE:HB2	2.56	0.41
1:C:426[A]:LEU:N	1:C:426[A]:LEU:HD23	2.36	0.40
1:C:350:MET:HA	1:C:353:MET:HE2	2.03	0.40

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	546/535 (102%)	533 (98%)	13 (2%)	0	100	100
1	C	542/535 (101%)	526 (97%)	16 (3%)	0	100	100
2	B	254/256 (99%)	246 (97%)	8 (3%)	0	100	100
2	D	254/256 (99%)	248 (98%)	5 (2%)	1 (0%)	39	34
All	All	1596/1582 (101%)	1553 (97%)	42 (3%)	1 (0%)	56	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	97	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/434 (101%)	427 (98%)	10 (2%)	58	62
1	C	430/434 (99%)	421 (98%)	9 (2%)	61	65
2	B	214/215 (100%)	212 (99%)	2 (1%)	84	89
2	D	213/215 (99%)	210 (99%)	3 (1%)	74	80
All	All	1294/1298 (100%)	1270 (98%)	24 (2%)	66	69

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	56	MET
1	A	74	LYS
1	A	137	ARG
1	A	222	MET
1	A	282	PHE
1	A	291	VAL
1	A	396	VAL
1	A	412	ASP
1	A	541	THR
2	B	35	ARG
2	B	104	TRP
1	C	48	THR
1	C	137	ARG
1	C	174	LEU
1	C	279	LEU
1	C	282	PHE
1	C	396	VAL
1	C	412	ASP
1	C	426[A]	LEU
1	C	426[B]	LEU
2	D	35	ARG
2	D	104	TRP
2	D	227	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 2 are modelled with single atom and 16 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	HEA	A	1	1	40,67,67	1.41	3 (7%)	41,103,103	1.77	14 (34%)
4	DMU	A	1005	-	22,22,34	0.54	0	27,27,45	0.99	2 (7%)
5	TRD	A	1009	-	6,6,12	0.25	0	5,5,11	0.38	0
5	TRD	A	1013	-	6,6,12	0.24	0	5,5,11	0.46	0
6	HEA	A	2[A]	1,13	40,67,67	1.41	4 (10%)	41,103,103	1.66	8 (19%)
6	HEA	A	2[B]	1,13	40,67,67	1.41	3 (7%)	41,103,103	1.73	12 (29%)
5	TRD	A	3	-	12,12,12	0.28	0	11,11,11	0.51	0
5	TRD	A	552	-	5,5,12	0.31	0	4,4,11	0.31	0
5	TRD	A	553	-	12,12,12	0.24	0	11,11,11	0.53	0
4	DMU	A	7	-	21,21,34	0.59	0	25,25,45	1.21	2 (8%)
4	DMU	B	1	-	34,34,34	0.48	0	45,45,45	0.89	2 (4%)
4	DMU	B	2	-	34,34,34	0.51	0	45,45,45	0.82	1 (2%)
11	HTH	B	286	-	9,9,9	0.38	0	8,10,10	0.82	0
4	DMU	B	3	-	34,34,34	0.54	0	45,45,45	0.60	0
5	TRD	B	4	-	7,7,12	0.25	0	6,6,11	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMU	B	6	-	24,24,34	0.54	0	35,35,45	0.69	0
6	HEA	C	1	1	40,67,67	1.37	3 (7%)	41,103,103	1.66	8 (19%)
4	DMU	C	10	-	34,34,34	0.58	0	45,45,45	0.83	1 (2%)
6	HEA	C	2[A]	1,13	40,67,67	1.41	5 (12%)	41,103,103	1.53	7 (17%)
6	HEA	C	2[B]	1,13	40,67,67	1.42	3 (7%)	41,103,103	1.63	10 (24%)
4	DMU	C	5	-	24,24,34	0.52	0	35,35,45	0.62	0
5	TRD	C	552	-	12,12,12	0.23	0	11,11,11	0.56	0
4	DMU	C	9	-	24,24,34	0.57	0	35,35,45	0.88	1 (2%)
5	TRD	D	14	-	6,6,12	0.25	0	5,5,11	0.35	0
5	TRD	D	3	-	12,12,12	0.20	0	11,11,11	0.66	0
4	DMU	D	4	-	24,24,34	0.51	0	35,35,45	0.62	0
4	DMU	D	8	-	24,24,34	0.52	0	35,35,45	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEA	A	1	1	2/2/7/16	0/24/76/76	0/0/8/8
4	DMU	A	1005	-	-	0/13/33/59	0/1/1/2
5	TRD	A	1009	-	-	0/4/4/10	0/0/0/0
5	TRD	A	1013	-	-	0/4/4/10	0/0/0/0
6	HEA	A	2[A]	1,13	3/3/7/16	0/24/76/76	0/0/8/8
6	HEA	A	2[B]	1,13	3/3/7/16	0/24/76/76	0/0/8/8
5	TRD	A	3	-	-	0/10/10/10	0/0/0/0
5	TRD	A	552	-	-	0/3/3/10	0/0/0/0
5	TRD	A	553	-	-	0/10/10/10	0/0/0/0
4	DMU	A	7	-	-	0/13/29/59	0/1/1/2
4	DMU	B	1	-	-	0/19/59/59	0/2/2/2
4	DMU	B	2	-	-	0/19/59/59	0/2/2/2
11	HTH	B	286	-	-	0/10/10/10	0/0/0/0
4	DMU	B	3	-	-	0/19/59/59	0/2/2/2
5	TRD	B	4	-	-	0/5/5/10	0/0/0/0
4	DMU	B	6	-	-	0/8/48/59	0/2/2/2
6	HEA	C	1	1	2/2/7/16	0/24/76/76	0/0/8/8
4	DMU	C	10	-	-	0/19/59/59	0/2/2/2
6	HEA	C	2[A]	1,13	3/3/7/16	0/24/76/76	0/0/8/8
6	HEA	C	2[B]	1,13	3/3/7/16	0/24/76/76	0/0/8/8
4	DMU	C	5	-	-	0/8/48/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRD	C	552	-	-	0/10/10/10	0/0/0/0
4	DMU	C	9	-	-	0/8/48/59	0/2/2/2
5	TRD	D	14	-	-	0/4/4/10	0/0/0/0
5	TRD	D	3	-	-	0/10/10/10	0/0/0/0
4	DMU	D	4	-	-	0/8/48/59	0/2/2/2
4	DMU	D	8	-	-	0/8/48/59	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	HEA	C3A-C2A	-4.91	1.33	1.40
6	C	2[B]	HEA	C3A-C2A	-4.74	1.34	1.40
6	A	2[B]	HEA	C3A-C2A	-4.71	1.34	1.40
6	A	2[A]	HEA	C3A-C2A	-4.63	1.34	1.40
6	C	1	HEA	C3A-C2A	-4.29	1.34	1.40
6	C	2[A]	HEA	C3A-C2A	-4.29	1.34	1.40
6	A	2[B]	HEA	C3C-C2C	-4.23	1.34	1.40
6	C	2[B]	HEA	C3C-C2C	-4.16	1.34	1.40
6	C	2[A]	HEA	C3C-C2C	-4.11	1.34	1.40
6	A	2[A]	HEA	C3C-C2C	-3.95	1.35	1.40
6	C	1	HEA	C3C-C2C	-3.79	1.35	1.40
6	A	1	HEA	C3C-C2C	-3.68	1.35	1.40
6	C	2[A]	HEA	C4B-NB	2.01	1.39	1.36
6	C	2[A]	HEA	C3A-CMA	2.17	1.51	1.46
6	A	2[A]	HEA	C3A-CMA	2.21	1.51	1.46
6	C	1	HEA	C3C-CAC	2.73	1.53	1.47
6	A	2[B]	HEA	C3C-CAC	2.86	1.53	1.47
6	C	2[B]	HEA	C3C-CAC	3.07	1.54	1.47
6	C	2[A]	HEA	C3C-CAC	3.07	1.54	1.47
6	A	1	HEA	C3C-CAC	3.13	1.54	1.47
6	A	2[A]	HEA	C3C-CAC	3.20	1.54	1.47

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2[A]	HEA	CAD-CBD-CGD	-4.72	104.10	112.75
6	A	2[B]	HEA	CAD-C3D-C4D	-4.55	122.07	127.01
6	A	1	HEA	C4B-C3B-C11	-4.40	122.23	127.01
6	C	2[B]	HEA	CAD-C3D-C4D	-4.37	122.26	127.01
6	A	2[A]	HEA	CAD-C3D-C4D	-4.29	122.35	127.01
6	C	2[A]	HEA	CAD-CBD-CGD	-3.78	105.83	112.75
6	C	1	HEA	CMC-C2C-C1C	-3.31	122.88	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1	HEA	C17-C18-C19	-3.16	120.89	127.76
6	A	2[B]	HEA	C3C-CAC-CBC	-3.10	119.98	126.32
6	C	1	HEA	C13-C14-C15	-3.06	121.11	127.76
6	C	1	HEA	C4B-C3B-C11	-2.99	123.76	127.01
6	C	2[B]	HEA	C17-C18-C19	-2.96	121.33	127.76
6	A	1	HEA	C13-C14-C15	-2.76	121.75	127.76
6	C	2[A]	HEA	C13-C12-C11	-2.72	110.89	114.51
6	C	1	HEA	CMB-C2B-C1B	-2.69	123.91	128.36
6	C	1	HEA	C13-C12-C11	-2.69	110.93	114.51
6	A	1	HEA	C13-C12-C11	-2.61	111.04	114.51
6	C	2[B]	HEA	C3C-CAC-CBC	-2.60	121.00	126.32
6	A	1	HEA	CMB-C2B-C1B	-2.60	124.06	128.36
4	A	7	DMU	C18-O16-C6	-2.60	109.40	113.94
6	C	2[B]	HEA	CBA-CAA-C2A	-2.55	107.96	112.53
6	A	2[B]	HEA	C17-C18-C19	-2.52	122.28	127.76
6	A	1	HEA	OMA-CMA-C3A	-2.49	120.09	125.11
6	A	2[B]	HEA	C3C-C4C-NC	-2.42	106.08	109.21
6	A	1	HEA	CMC-C2C-C1C	-2.38	124.42	128.36
6	C	2[A]	HEA	CMB-C2B-C1B	-2.37	124.44	128.36
6	A	2[B]	HEA	OMA-CMA-C3A	-2.37	120.32	125.11
6	A	2[A]	HEA	OMA-CMA-C3A	-2.36	120.35	125.11
6	C	1	HEA	CAD-CBD-CGD	-2.35	108.44	112.75
6	C	2[A]	HEA	C3C-CAC-CBC	-2.33	121.55	126.32
6	A	2[A]	HEA	CMC-C2C-C1C	-2.29	124.58	128.36
6	C	2[B]	HEA	OMA-CMA-C3A	-2.25	120.56	125.11
6	A	2[B]	HEA	CAD-CBD-CGD	-2.25	108.62	112.75
6	C	2[B]	HEA	CMC-C2C-C1C	-2.24	124.67	128.36
6	A	2[B]	HEA	CMC-C2C-C1C	-2.23	124.67	128.36
6	C	1	HEA	CAA-C2A-C1A	-2.23	124.59	127.01
6	C	2[B]	HEA	C3A-C4A-NA	-2.19	106.81	110.94
4	A	1005	DMU	C18-O16-C6	-2.19	110.12	113.94
6	A	1	HEA	C3A-C4A-NA	-2.18	106.83	110.94
6	A	2[B]	HEA	C13-C14-C15	-2.18	123.02	127.76
6	A	1	HEA	CAA-C2A-C1A	-2.18	124.64	127.01
6	A	1	HEA	C3B-C4B-NB	-2.18	106.83	110.94
4	B	1	DMU	C10-O7-C3	-2.16	112.36	118.01
6	A	1	HEA	C12-C11-C3B	-2.13	108.19	112.59
6	A	2[B]	HEA	CBA-CAA-C2A	-2.11	108.75	112.53
6	C	2[B]	HEA	C13-C14-C15	-2.09	123.21	127.76
4	C	9	DMU	C10-O7-C3	-2.09	112.54	118.01
6	C	2[A]	HEA	C3A-C4A-NA	-2.07	107.04	110.94
6	A	1	HEA	C27-C19-C18	-2.06	119.46	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2[B]	HEA	C3A-C4A-NA	-2.06	107.06	110.94
6	A	2[A]	HEA	CMB-C2B-C1B	-2.05	124.97	128.36
6	A	2[A]	HEA	CAA-CBA-CGA	-2.03	109.03	112.75
4	C	10	DMU	C10-O1-C9	2.02	117.67	113.75
6	A	1	HEA	C26-C15-C16	2.04	118.52	115.41
4	B	1	DMU	O2-C8-C9	2.05	114.66	109.24
6	C	2[A]	HEA	C26-C15-C16	2.34	118.98	115.41
6	C	2[B]	HEA	CBD-CAD-C3D	2.52	117.04	112.53
4	A	1005	DMU	O16-C6-C1	2.59	111.31	108.04
6	C	1	HEA	C27-C19-C20	2.66	119.48	115.41
6	A	2[A]	HEA	CBD-CAD-C3D	2.80	117.55	112.53
6	C	2[B]	HEA	C26-C15-C16	2.93	119.88	115.41
6	A	2[B]	HEA	C26-C15-C16	2.95	119.92	115.41
6	A	2[A]	HEA	C27-C19-C20	3.13	120.18	115.41
6	A	1	HEA	C27-C19-C20	3.18	120.26	115.41
6	C	2[A]	HEA	C27-C19-C20	3.30	120.45	115.41
6	A	2[B]	HEA	CBD-CAD-C3D	3.31	118.46	112.53
4	B	2	DMU	O16-C6-C1	3.34	112.25	108.04
4	A	7	DMU	O16-C6-C1	4.23	113.38	108.04

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	2[A]	HEA	NB
6	C	2[A]	HEA	NA
6	C	2[A]	HEA	ND
6	C	2[B]	HEA	ND
6	C	2[B]	HEA	NA
6	C	2[B]	HEA	NB
6	A	1	HEA	ND
6	A	1	HEA	NB
6	C	1	HEA	ND
6	C	1	HEA	NB
6	A	2[B]	HEA	ND
6	A	2[B]	HEA	NA
6	A	2[B]	HEA	NB
6	A	2[A]	HEA	ND
6	A	2[A]	HEA	NA
6	A	2[A]	HEA	NB

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1	HEA	3	0
4	A	1005	DMU	2	0
6	A	2[A]	HEA	7	0
6	A	2[B]	HEA	9	0
5	A	3	TRD	1	0
5	A	553	TRD	1	0
6	C	1	HEA	6	0
4	C	10	DMU	1	0
6	C	2[A]	HEA	7	0
6	C	2[B]	HEA	8	0
5	C	552	TRD	1	0
4	C	9	DMU	1	0
4	D	8	DMU	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	535/535 (100%)	0.21	40 (7%) 17 23	24, 35, 57, 81	0
1	C	531/535 (99%)	0.87	106 (19%) 1 2	30, 52, 76, 88	0
2	B	256/256 (100%)	-0.11	7 (2%) 58 67	23, 39, 55, 59	0
2	D	256/256 (100%)	0.08	14 (5%) 29 39	30, 44, 64, 72	0
All	All	1578/1582 (99%)	0.36	167 (10%) 8 13	23, 42, 67, 88	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	7.6
2	D	284	HIS	7.1
1	C	222	MET	6.8
2	B	56	TRP	6.3
1	A	20	TRP	6.1
1	C	21	PHE	5.7
1	C	217	ALA	5.3
1	C	22	MET	5.1
1	A	81	TRP	5.0
1	C	81	TRP	4.9
1	C	290	ILE	4.9
1	C	259	PHE	4.8
1	C	549	HIS	4.8
1	C	287	VAL	4.7
1	C	423[A]	VAL	4.7
1	C	218	PRO	4.7
1	A	22	MET	4.7
2	D	81	TRP	4.6
1	C	73	VAL	4.6
1	C	23	SER	4.5
1	A	221	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	424[A]	MET	4.2
1	C	172	TRP	4.1
1	C	71	GLY	4.1
1	C	138	MET	4.1
1	C	77	PHE	4.0
1	C	417	VAL	3.9
1	C	223	HIS	3.9
1	A	172	TRP	3.9
1	A	423[A]	VAL	3.9
1	A	424[A]	MET	3.9
2	D	96	HIS	3.9
1	C	289	ILE	3.8
1	A	549	HIS	3.8
1	C	137	ARG	3.8
1	A	220	MET	3.8
2	D	56	TRP	3.8
1	C	130	ALA	3.7
1	C	221	THR	3.7
1	C	520	THR	3.7
1	C	280	TRP	3.6
1	C	426[A]	LEU	3.6
2	D	87	ARG	3.6
1	C	318	TYR	3.6
1	A	19	ARG	3.6
2	D	98	SER	3.6
1	A	551	PHE	3.5
1	C	425[A]	SER	3.5
1	A	420	PHE	3.5
1	C	269	GLY	3.5
1	C	74	LYS	3.5
1	C	111	VAL	3.5
1	C	550	THR	3.5
1	C	131	PRO	3.4
1	C	428[A]	ALA	3.4
1	C	99	ILE	3.4
1	C	314	LEU	3.4
1	A	259	PHE	3.4
1	A	17	PHE	3.3
1	A	287	VAL	3.3
1	A	222	MET	3.3
1	A	426[A]	LEU	3.3
2	D	99	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	75	GLY	3.3
1	A	425[A]	SER	3.2
2	D	100	LEU	3.2
2	B	284	HIS	3.2
1	C	414	TYR	3.2
1	A	417	VAL	3.2
1	C	76	PHE	3.2
1	C	420	PHE	3.2
1	A	173	VAL	3.1
1	C	481	ARG	3.1
1	C	78	GLN	3.1
1	C	173	VAL	3.1
1	C	219	GLY	3.1
2	D	102	ILE	3.1
1	C	268	GLY	3.1
1	C	279	LEU	3.0
1	C	132	ALA	3.0
1	C	213	LEU	3.0
1	C	267	SER	3.0
1	A	428[A]	ALA	3.0
1	C	107	MET	3.0
1	C	69	GLU	2.9
1	C	283	GLY	2.9
1	A	99	ILE	2.9
1	C	416	VAL	2.9
1	C	422[A]	TYR	2.9
1	C	139	ASN	2.8
2	D	82	ARG	2.8
1	C	451	TRP	2.8
1	C	429[A]	VAL	2.8
1	A	401	LEU	2.7
1	C	261	THR	2.7
1	C	103	GLY	2.7
1	A	217	ALA	2.7
1	C	288	TYR	2.7
2	D	83	PHE	2.7
1	C	220	MET	2.7
1	A	289	ILE	2.7
1	C	112	ILE	2.7
1	A	18	THR	2.7
1	C	110	VAL	2.6
1	A	69	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	99	PRO	2.6
1	A	73	VAL	2.6
2	B	87	ARG	2.6
2	D	78	TYR	2.6
1	C	106	MET	2.6
1	C	70	SER	2.5
1	C	359[A]	THR	2.5
1	C	468	PHE	2.5
1	C	291	VAL	2.5
1	C	480	PRO	2.5
1	A	104	ILE	2.5
1	C	397	THR	2.5
1	A	71	GLY	2.5
1	C	100	THR	2.5
2	B	81	TRP	2.5
1	A	107	MET	2.4
1	C	214	ASN	2.4
1	C	517	TYR	2.4
1	C	530	TYR	2.4
1	C	418	ALA	2.4
1	C	446	ARG	2.4
2	D	124	PHE	2.4
1	C	427[A]	GLY	2.4
1	C	312	GLY	2.4
1	C	134	ALA	2.4
1	C	391	PHE	2.4
2	D	86	LYS	2.4
1	A	394	GLY	2.3
1	C	210	THR	2.3
1	C	432	ILE	2.3
1	C	164	GLY	2.3
1	C	270	GLY	2.3
1	C	394	GLY	2.3
1	C	263	PHE	2.3
1	C	246	LEU	2.3
2	B	98	SER	2.3
1	C	136	PRO	2.3
1	C	285	PRO	2.2
1	A	74	LYS	2.2
2	B	102	ILE	2.2
1	A	427[A]	GLY	2.2
1	A	21	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	526	THR	2.2
1	C	371	TRP	2.2
1	C	292	LEU	2.2
1	C	282	PHE	2.2
1	A	260	GLY	2.2
1	A	77	PHE	2.2
1	A	171	GLY	2.2
1	C	482	ARG	2.2
1	C	412	ASP	2.2
1	C	533	GLU	2.2
1	C	237	TRP	2.2
1	C	311	PHE	2.2
1	C	413	THR	2.1
1	C	144	TRP	2.1
1	C	400	VAL	2.1
1	C	24	THR	2.1
1	A	297	ILE	2.1
1	C	72	LEU	2.1
1	A	214	ASN	2.1
1	C	262	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	DMU	C	9	23/33	0.50	0.36	8.70	85,86,89,89	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMU	B	2	33/33	0.88	0.16	8.39	49,54,56,57	33
5	TRD	B	4	8/13	0.87	0.31	5.57	35,36,37,37	0
11	HTH	B	286	10/10	0.80	0.33	4.57	56,60,61,61	0
5	TRD	A	1013	7/13	0.68	0.26	4.05	54,56,57,57	0
4	DMU	A	1005	22/33	0.79	0.14	4.02	44,49,53,54	22
5	TRD	A	3	13/13	0.84	0.28	3.47	46,49,53,54	0
4	DMU	C	10	33/33	0.87	0.18	3.30	73,74,76,76	0
8	MG	A	6	1/1	0.99	0.22	3.21	13,13,13,13	0
4	DMU	B	3	33/33	0.88	0.27	2.92	73,78,82,83	0
5	TRD	D	3	13/13	0.85	0.29	2.66	55,58,61,61	0
3	OH	A	802	1/1	0.98	0.30	2.44	8,8,8,8	1
8	MG	C	6	1/1	0.99	0.24	1.58	18,18,18,18	0
4	DMU	B	1	33/33	0.94	0.11	1.54	26,35,46,48	0
5	TRD	D	14	7/13	0.77	0.16	1.27	65,65,65,65	0
4	DMU	A	7	21/33	0.80	0.18	1.05	43,59,70,72	0
6	HEA	A	2[B]	60/60	0.96	0.24	0.92	30,33,41,41	60
6	HEA	A	2[A]	60/60	0.96	0.24	0.78	21,22,30,32	60
5	TRD	A	1009	7/13	0.84	0.15	0.74	57,58,58,58	0
6	HEA	A	1	60/60	0.98	0.20	0.32	21,25,30,32	0
6	HEA	C	2[B]	60/60	0.96	0.21	0.16	35,40,48,48	60
6	HEA	C	1	60/60	0.96	0.22	0.13	31,34,47,47	0
9	CA	A	554	1/1	1.00	0.09	0.11	27,27,27,27	0
6	HEA	C	2[A]	60/60	0.96	0.21	-0.01	25,28,33,34	60
7	CU1	B	288	1/1	1.00	0.12	-0.01	26,26,26,26	0
7	CU1	D	287	1/1	1.00	0.11	-0.43	32,32,32,32	0
12	CD	B	9	1/1	0.99	0.13	-0.49	39,39,39,39	1
7	CU1	D	286	1/1	1.00	0.12	-0.57	33,33,33,33	0
7	CU1	B	287	1/1	1.00	0.10	-1.17	25,25,25,25	0
12	CD	D	288	1/1	0.99	0.07	-1.40	40,40,40,40	0
10	CL	C	554	1/1	0.89	0.18	-2.11	68,68,68,68	0
12	CD	B	8	1/1	0.99	0.07	-2.43	41,41,41,41	0
10	CL	A	10	1/1	0.97	0.04	-2.88	41,41,41,41	0
12	CD	D	9	1/1	0.96	0.07	-3.23	63,63,63,63	1
9	CA	C	7	1/1	0.98	0.04	-3.58	38,38,38,38	0
4	DMU	D	4	23/33	0.86	0.23	-	91,91,91,91	23
3	OH	C	802	1/1	0.97	0.84	-	21,21,21,21	1
5	TRD	C	552	13/13	0.75	0.19	-	80,82,83,84	0
4	DMU	C	5	23/33	0.80	0.24	-	97,98,98,99	23
4	DMU	D	8	23/33	0.78	0.23	-	89,90,93,93	23
7	CU1	C	553	1/1	0.98	0.15	-	45,45,45,45	0
7	CU1	A	5	1/1	0.99	0.17	-	37,37,37,37	0
4	DMU	B	6	23/33	0.81	0.19	-	76,77,78,78	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TRD	A	552	6/13	0.75	0.18	-	62,63,63,63	0
5	TRD	A	553	13/13	0.78	0.25	-	71,71,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.