



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:17 AM GMT

PDB ID : 3OM3  
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with K362M mutation in the reduced state  
Authors : Liu, J.; Qin, L.; Ferguson-Miller, S.  
Deposited on : 2010-08-26  
Resolution : 2.60 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

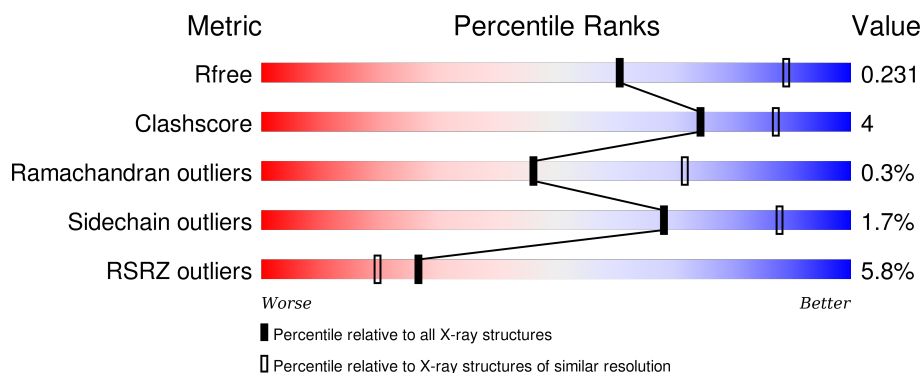
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>5%</div> <div>88%</div> <div>11%</div> </div>
1	C	535	<div> <div>9%</div> <div>87%</div> <div>12%</div> </div>
2	B	256	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>
2	D	256	<div> <div>4%</div> <div>91%</div> <div>8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMU	A	1005	-	-	-	X
3	DMU	C	10	-	-	-	X
3	DMU	C	9	X	-	-	-
4	TRD	A	1013	-	-	-	X
4	TRD	B	4	-	-	-	X
4	TRD	D	14	-	-	-	X
5	HEA	A	1	X	-	-	-
5	HEA	A	2	X	-	-	-
5	HEA	C	1	X	-	-	-
5	HEA	C	2	X	-	-	-
9	HTH	B	286	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13203 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	0	0
			4166	2790	655	689	32			
1	C	531	Total	C	N	O	S	0	0	0
			4095	2742	638	685	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	MET	LYS	ENGINEERED MUTATION	UNP Q3J5A7
C	362	MET	LYS	ENGINEERED MUTATION	UNP Q3J5A7

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

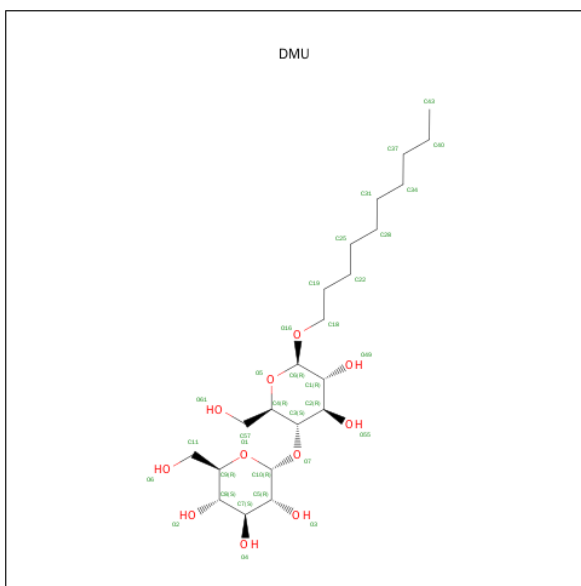
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2014	1314	332	362	6			
2	D	256	Total	C	N	O	S	0	0	0
			2013	1313	331	363	6			

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

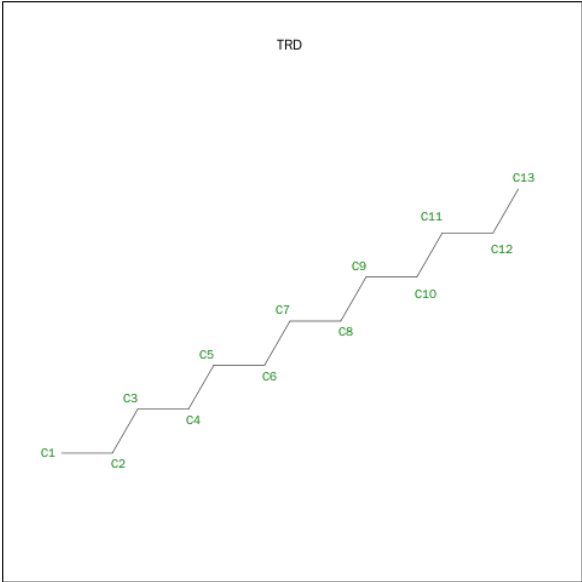
- Molecule 3 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code:

DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



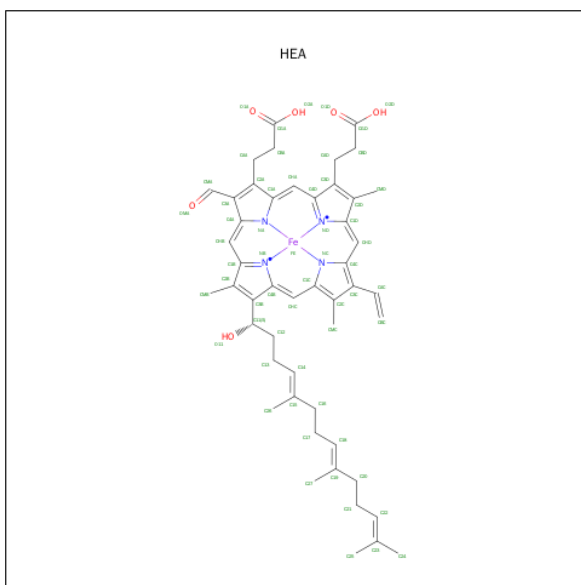
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 22	C 16	O 6	0	0
3	A	1	Total 22	C 16	O 6	0	0
3	B	1	Total 33	C 22	O 11	0	0
3	B	1	Total 33	C 22	O 11	0	0
3	B	1	Total 33	C 22	O 11	0	0
3	B	1	Total 23	C 12	O 11	0	0
3	C	1	Total 33	C 22	O 11	0	0
3	C	1	Total 23	C 12	O 11	0	0
3	C	1	Total 12	C 6	O 6	0	0
3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

- Molecule 4 is TRIDECANE (three-letter code: TRD) (formula:  $\text{C}_{13}\text{H}_{28}$ ).



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

- Molecule 5 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
5	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
5	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
5	C	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
5	C	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

- Molecule 6 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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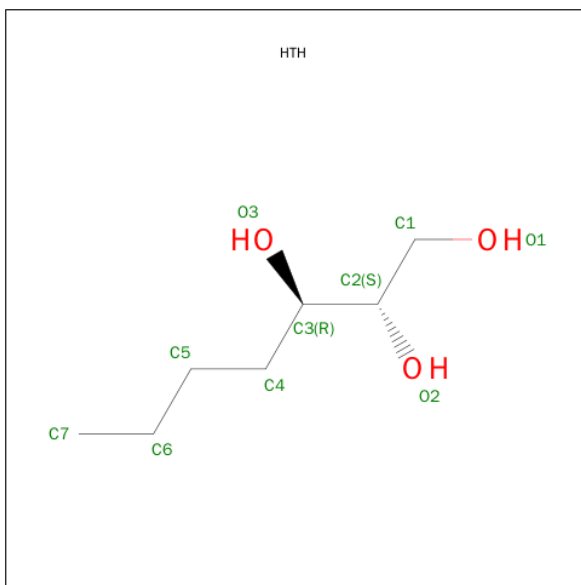
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 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
9	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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



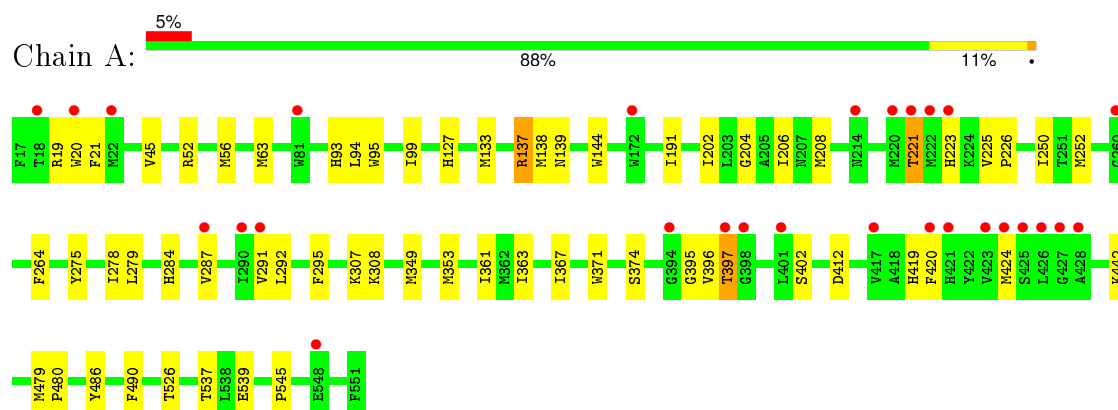
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	91	Total 91	O 91	0	0
11	B	91	Total 91	O 91	0	0
11	C	46	Total 46	O 46	0	0
11	D	54	Total 54	O 54	0	0

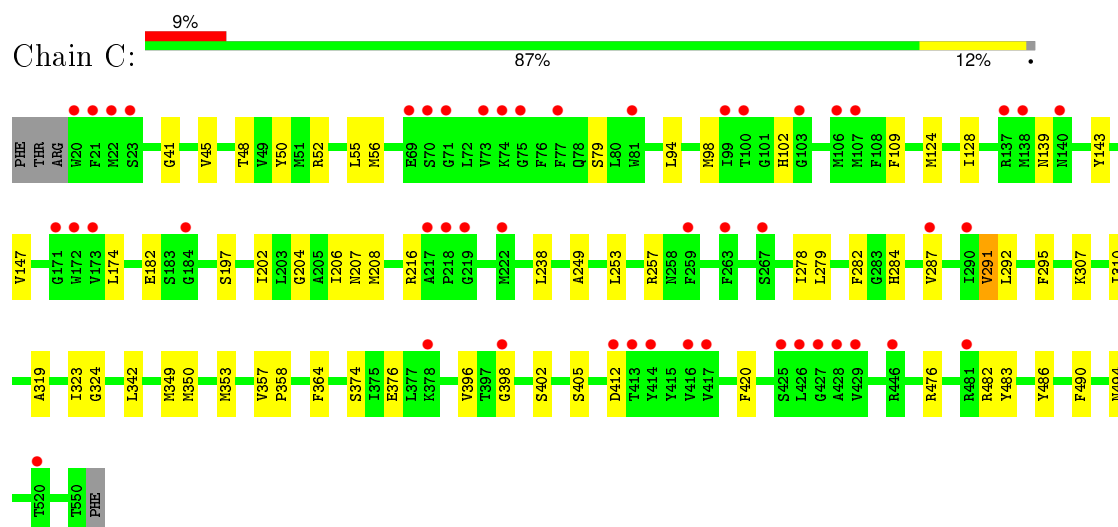
### 3 Residue-property plots [i](#)

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.

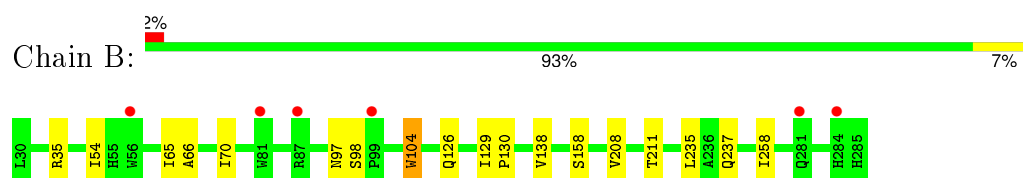
- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I



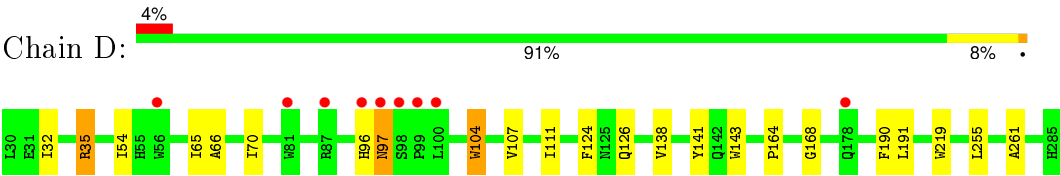
- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I



- 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, $\alpha$ , $\beta$ , $\gamma$	124.65Å 132.37Å 178.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.46 – 2.60 40.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.46-2.60) 95.7 (40.46-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.198 , 0.229 0.199 , 0.231	Depositor DCC
$R_{free}$ test set	2630 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 87092 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, CA, 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	0.52	0/4320	0.56	0/5902
1	C	0.47	0/4244	0.52	0/5803
2	B	0.51	0/2076	0.57	0/2843
2	D	0.47	0/2074	0.51	0/2840
All	All	0.49	0/12714	0.54	0/17388

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	4166	0	4051	39	0
1	C	4095	0	3967	39	0
2	B	2014	0	1963	10	0
2	D	2013	0	1964	17	0
3	A	44	0	62	1	0
3	B	122	0	147	0	0
3	C	68	0	74	1	0
3	D	46	0	42	1	0
4	A	47	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	9	0	17	0	0
4	C	26	0	56	1	0
4	D	7	0	13	0	0
5	A	120	0	108	10	0
5	C	120	0	108	7	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	B	10	0	16	0	0
10	B	2	0	0	0	0
10	D	2	0	0	0	0
11	A	91	0	0	0	0
11	B	91	0	0	0	0
11	C	46	0	0	0	0
11	D	54	0	0	0	0
All	All	13203	0	12680	103	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 4.

All (103) 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:21:PHE:HB3	1:A:144:TRP:HZ2	1.35	0.89
5:C:1:HEA:HBC1	5:C:1:HEA:HMC1	1.54	0.87
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.21	0.75
5:A:2:HEA:HMD1	5:A:2:HEA:HBD2	1.68	0.75
2:B:66:ALA:O	2:B:70:ILE:HG12	1.88	0.74
1:A:138:MET:HE3	1:A:206:ILE:HB	1.71	0.72
1:C:56:MET:HE1	3:C:10:DMU:H6	1.72	0.71
1:A:397:THR:CG2	1:A:419:HIS:HB2	2.20	0.70
5:A:1:HEA:HBC1	5:A:1:HEA:HMC1	1.73	0.68
2:B:54:ILE:HD11	2:B:126:GLN:NE2	2.11	0.66
1:A:396:VAL:HB	2:B:65:ILE:HB	1.81	0.63
1:A:204:GLY:O	1:A:208:MET:HG2	2.02	0.60
1:C:319:ALA:O	1:C:323:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:HIS:CD2	1:A:284:HIS:C	2.76	0.59
1:A:138:MET:CE	1:A:206:ILE:HB	2.33	0.58
1:A:397:THR:HG22	1:A:419:HIS:ND1	2.19	0.58
1:A:397:THR:HG22	1:A:419:HIS:HD1	1.69	0.57
1:A:56:MET:HE1	3:A:1005:DMU:H6	1.86	0.57
1:C:204:GLY:O	1:C:208:MET:HG2	2.05	0.56
2:D:66:ALA:O	2:D:70:ILE:HG12	2.05	0.56
1:A:307:LYS:HE2	1:A:374:SER:HB3	1.88	0.55
2:D:32:ILE:HG22	2:D:35:ARG:HD2	1.88	0.55
1:C:405:SER:O	2:D:54:ILE:HD12	2.07	0.53
1:C:287:VAL:HB	5:C:2:HEA:HAC	1.91	0.53
1:C:50:TYR:OH	1:C:79:SER:HB2	2.08	0.53
2:D:54:ILE:HD11	2:D:126:GLN:NE2	2.24	0.53
1:A:287:VAL:HB	5:A:2:HEA:HAC	1.91	0.52
1:C:396:VAL:HB	2:D:65:ILE:HB	1.91	0.52
1:A:221:THR:HG22	1:A:223:HIS:H	1.74	0.52
1:C:253:LEU:O	1:C:257:ARG:HG3	2.10	0.52
1:A:45:VAL:HG21	5:A:1:HEA:H171	1.93	0.51
1:A:63:MET:HG2	1:A:94:LEU:HD23	1.91	0.51
3:D:8:DMU:H35	3:D:8:DMU:H29	1.91	0.50
1:A:397:THR:HG21	1:A:419:HIS:HB2	1.92	0.50
2:B:211:THR:HB	2:B:235:LEU:HD12	1.92	0.49
1:A:402:SER:HA	5:A:2:HEA:OMA	2.12	0.49
1:A:442:LYS:O	1:A:545:PRO:HA	2.13	0.49
1:C:402:SER:HA	5:C:2:HEA:OMA	2.12	0.48
2:D:104:TRP:CD1	2:D:104:TRP:C	2.86	0.48
1:C:349:MET:O	1:C:353:MET:HG3	2.13	0.48
1:A:291:VAL:HG13	5:A:2:HEA:HBC2	1.96	0.48
1:C:350:MET:HG2	1:C:353:MET:CE	2.44	0.48
1:A:292:LEU:O	1:A:295:PHE:HB2	2.14	0.47
2:B:129:ILE:HD13	2:B:237:GLN:HB2	1.96	0.47
1:C:342:LEU:HD21	2:D:124:PHE:CD2	2.49	0.47
1:C:349:MET:HG3	1:C:402:SER:O	2.13	0.47
2:D:107:VAL:O	2:D:111:ILE:HG12	2.14	0.47
1:C:476:ARG:HH21	4:C:3:TRD:H21	1.80	0.47
1:C:94:LEU:O	1:C:98:MET:HG2	2.15	0.47
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.50	0.47
1:C:284:HIS:CD2	1:C:284:HIS:C	2.88	0.47
1:C:249:ALA:HB2	1:C:278:ILE:HG22	1.97	0.46
5:A:2:HEA:H212	5:A:2:HEA:H18	1.62	0.46
1:A:95:TRP:CZ2	1:A:99:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:THR:CG2	1:C:102:HIS:CE1	3.00	0.45
1:C:420:PHE:HB2	5:C:2:HEA:HMD3	1.97	0.45
2:D:190:PHE:O	2:D:191:LEU:HB2	2.17	0.45
2:D:141:TYR:O	2:D:143:TRP:HA	2.16	0.45
2:D:96:HIS:O	2:D:97:ASN:HB2	2.16	0.45
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.51	0.45
2:D:164:PRO:HA	2:D:168:GLY:O	2.17	0.45
2:B:129:ILE:HA	2:B:130:PRO:HD3	1.82	0.44
1:A:93:HIS:N	2:B:258:ILE:HG13	2.32	0.44
1:C:55:LEU:O	1:C:494:ASN:HB3	2.17	0.44
1:A:264:PHE:CE1	1:A:275:TYR:HB2	2.53	0.44
2:B:138:VAL:HG23	2:B:208:VAL:HG13	1.98	0.44
1:A:191:ILE:HG23	1:A:250:ILE:HD12	2.00	0.44
1:C:143:TYR:O	1:C:147:VAL:HG23	2.18	0.44
1:C:41:GLY:O	1:C:45:VAL:HG23	2.18	0.44
2:B:104:TRP:CD1	2:B:104:TRP:C	2.92	0.43
1:A:349:MET:HG2	1:A:353:MET:HE2	2.00	0.43
1:C:292:LEU:O	1:C:295:PHE:HB2	2.18	0.43
1:A:424:MET:HE2	5:A:2:HEA:HMD3	2.00	0.43
1:C:139:ASN:HB2	1:C:207:ASN:ND2	2.33	0.43
1:A:486:TYR:CD2	1:A:490:PHE:HB2	2.53	0.43
2:B:54:ILE:HD11	2:B:126:GLN:HE21	1.83	0.43
1:A:252:MET:HE1	1:A:278:ILE:HD13	2.01	0.42
1:C:398:GLY:O	5:C:2:HEA:HMB3	2.19	0.42
1:C:48:THR:O	1:C:52:ARG:HG2	2.19	0.42
2:D:35:ARG:HG2	2:D:35:ARG:O	2.17	0.42
1:C:238:LEU:HD21	1:C:324:GLY:CA	2.49	0.42
1:C:124:MET:O	1:C:128:ILE:HG12	2.20	0.41
1:C:486:TYR:CD2	1:C:490:PHE:HB2	2.56	0.41
1:C:357:VAL:HB	1:C:358:PRO:CD	2.50	0.41
1:A:202:ILE:O	1:A:206:ILE:HG12	2.20	0.41
1:C:291:VAL:HG13	5:C:2:HEA:HBC2	2.02	0.41
1:A:479:MET:HA	1:A:480:PRO:HD3	1.89	0.41
1:A:420:PHE:HB2	5:A:2:HEA:HMD3	2.03	0.41
1:C:202:ILE:O	1:C:206:ILE:HG12	2.20	0.41
1:C:182:GLU:O	1:C:257:ARG:NH1	2.53	0.41
1:A:537:THR:OG1	1:A:539:GLU:OE1	2.32	0.41
1:A:225:VAL:HA	1:A:226:PRO:HD3	1.96	0.41
1:A:308:LYS:HE3	1:A:371:TRP:O	2.21	0.41
1:C:128:ILE:HB	1:C:216:ARG:HG2	2.03	0.40
1:C:483:TYR:CZ	2:D:261:ALA:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ARG:HD3	2:D:255:LEU:HB2	2.03	0.40
1:A:363:ILE:O	1:A:367:ILE:HG13	2.21	0.40
1:C:307:LYS:HE2	1:C:374:SER:HB3	2.02	0.40
1:A:395:GLY:HA3	5:A:2:HEA:C15	2.52	0.40
5:C:2:HEA:H212	5:C:2:HEA:H18	1.54	0.40
1:A:133:MET:HG3	1:A:139:ASN:ND2	2.36	0.40
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.57	0.40
1:A:137:ARG:HB2	1:A:137:ARG:HE	1.80	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	533/535 (100%)	513 (96%)	18 (3%)	2 (0%)	39	65
1	C	529/535 (99%)	513 (97%)	16 (3%)	0	100	100
2	B	254/256 (99%)	244 (96%)	9 (4%)	1 (0%)	39	65
2	D	254/256 (99%)	245 (96%)	8 (3%)	1 (0%)	39	65
All	All	1570/1582 (99%)	1515 (96%)	51 (3%)	4 (0%)	46	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	20	TRP
2	D	97	ASN
2	B	97	ASN

### 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	424/435 (98%)	415 (98%)	9 (2%)	61	85
1	C	415/435 (95%)	408 (98%)	7 (2%)	68	88
2	B	212/215 (99%)	208 (98%)	4 (2%)	65	86
2	D	212/215 (99%)	210 (99%)	2 (1%)	84	95
All	All	1263/1300 (97%)	1241 (98%)	22 (2%)	68	88

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	127	HIS
1	A	137	ARG
1	A	221	THR
1	A	279	LEU
1	A	361	ILE
1	A	397	THR
1	A	412	ASP
1	A	526	THR
2	B	35	ARG
2	B	98	SER
2	B	104	TRP
2	B	158	SER
1	C	174	LEU
1	C	279	LEU
1	C	282	PHE
1	C	291	VAL
1	C	310	ILE
1	C	376	GLU
1	C	412	ASP
2	D	35	ARG
2	D	104	TRP

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

Mol	Chain	Res	Type
1	A	447	GLN

### 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 39 ligands modelled in this entry, 14 are monoatomic - leaving 25 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	$\# Z  > 2$
5	HEA	A	1	1	40,67,67	1.41	4 (10%)	41,103,103	1.53	8 (19%)
3	DMU	A	1005	-	22,22,34	0.53	0	27,27,45	0.84	1 (3%)
4	TRD	A	1009	-	6,6,12	0.28	0	5,5,11	0.37	0
4	TRD	A	1013	-	6,6,12	0.34	0	5,5,11	0.28	0
4	TRD	A	1015	-	6,6,12	0.34	0	5,5,11	0.31	0
5	HEA	A	2	1	40,67,67	1.41	4 (10%)	41,103,103	1.61	8 (19%)
4	TRD	A	3	-	12,12,12	0.29	0	11,11,11	0.51	0
4	TRD	A	552	-	12,12,12	0.30	0	11,11,11	0.39	0
3	DMU	A	7	-	22,22,34	0.64	1 (4%)	27,27,45	0.86	1 (3%)
3	DMU	B	1	-	34,34,34	0.58	1 (2%)	45,45,45	1.13	3 (6%)
3	DMU	B	2	-	34,34,34	0.54	1 (2%)	45,45,45	0.86	2 (4%)
9	HTH	B	286	-	9,9,9	0.42	0	8,10,10	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMU	B	3	-	34,34,34	0.57	0	45,45,45	0.60	0
4	TRD	B	4	-	8,8,12	0.27	0	7,7,11	0.47	0
3	DMU	B	6	-	24,24,34	0.58	0	35,35,45	0.72	0
5	HEA	C	1	1	40,67,67	1.40	4 (10%)	41,103,103	1.51	9 (21%)
3	DMU	C	10	-	34,34,34	0.54	0	45,45,45	0.81	1 (2%)
5	HEA	C	2	1	40,67,67	1.36	4 (10%)	41,103,103	1.71	11 (26%)
4	TRD	C	3	-	12,12,12	0.26	0	11,11,11	0.54	0
3	DMU	C	5	-	24,24,34	0.55	0	35,35,45	0.72	0
4	TRD	C	552	-	12,12,12	0.28	0	11,11,11	0.48	0
3	DMU	C	9	-	12,12,34	0.57	0	17,17,45	0.46	0
4	TRD	D	14	-	6,6,12	0.27	0	5,5,11	0.39	0
3	DMU	D	4	-	24,24,34	0.55	0	35,35,45	0.85	1 (2%)
3	DMU	D	8	-	24,24,34	0.58	0	35,35,45	0.60	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
5	HEA	A	1	1	2/2/7/16	0/24/76/76	0/0/8/8
3	DMU	A	1005	-	-	0/13/33/59	0/1/1/2
4	TRD	A	1009	-	-	0/4/4/10	0/0/0/0
4	TRD	A	1013	-	-	0/4/4/10	0/0/0/0
4	TRD	A	1015	-	-	0/4/4/10	0/0/0/0
5	HEA	A	2	1	3/3/7/16	0/24/76/76	0/0/8/8
4	TRD	A	3	-	-	0/10/10/10	0/0/0/0
4	TRD	A	552	-	-	0/10/10/10	0/0/0/0
3	DMU	A	7	-	-	0/13/33/59	0/1/1/2
3	DMU	B	1	-	-	0/19/59/59	0/2/2/2
3	DMU	B	2	-	-	0/19/59/59	0/2/2/2
9	HTH	B	286	-	-	0/10/10/10	0/0/0/0
3	DMU	B	3	-	-	0/19/59/59	0/2/2/2
4	TRD	B	4	-	-	0/6/6/10	0/0/0/0
3	DMU	B	6	-	-	0/8/48/59	0/2/2/2
5	HEA	C	1	1	2/2/7/16	0/24/76/76	0/0/8/8
3	DMU	C	10	-	-	0/19/59/59	0/2/2/2
5	HEA	C	2	1	3/3/7/16	0/24/76/76	0/0/8/8
4	TRD	C	3	-	-	0/10/10/10	0/0/0/0
3	DMU	C	5	-	-	0/8/48/59	0/2/2/2
4	TRD	C	552	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMU	C	9	-	1/1/5/10	0/2/22/59	0/1/1/2
4	TRD	D	14	-	-	0/4/4/10	0/0/0/0
3	DMU	D	4	-	-	0/8/48/59	0/2/2/2
3	DMU	D	8	-	-	0/8/48/59	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	HEA	C3A-C2A	-4.75	1.34	1.40
5	A	1	HEA	C3A-C2A	-4.72	1.34	1.40
5	A	2	HEA	C3C-C2C	-4.71	1.34	1.40
5	C	2	HEA	C3C-C2C	-4.30	1.34	1.40
5	A	2	HEA	C3A-C2A	-4.14	1.34	1.40
5	C	2	HEA	C3A-C2A	-3.99	1.35	1.40
5	A	1	HEA	C3C-C2C	-3.65	1.35	1.40
5	C	1	HEA	C3C-C2C	-3.47	1.35	1.40
3	B	2	DMU	O16-C6	2.02	1.43	1.40
3	B	1	DMU	O16-C6	2.10	1.43	1.40
5	C	1	HEA	C3A-CMA	2.10	1.51	1.46
3	A	7	DMU	O16-C6	2.14	1.44	1.40
5	A	1	HEA	C4B-NB	2.16	1.39	1.36
5	C	2	HEA	C3A-CMA	2.32	1.51	1.46
5	A	2	HEA	C3A-CMA	2.33	1.52	1.46
5	C	2	HEA	C3C-CAC	2.83	1.53	1.47
5	A	2	HEA	C3C-CAC	2.83	1.53	1.47
5	C	1	HEA	C3C-CAC	3.01	1.54	1.47
5	A	1	HEA	C3C-CAC	3.24	1.54	1.47

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2	HEA	CAD-C3D-C4D	-4.18	122.47	127.01
5	C	2	HEA	CAD-C3D-C4D	-3.56	123.14	127.01
5	C	1	HEA	C4B-C3B-C11	-3.54	123.17	127.01
5	C	2	HEA	C3C-CAC-CBC	-3.47	119.22	126.32
5	C	2	HEA	CAD-CBD-CGD	-3.04	107.17	112.75
5	A	2	HEA	C3C-CAC-CBC	-2.82	120.55	126.32
5	C	1	HEA	C13-C12-C11	-2.77	110.83	114.51
5	A	1	HEA	C4B-C3B-C11	-2.75	124.02	127.01
5	A	1	HEA	C17-C18-C19	-2.69	121.91	127.76
5	A	1	HEA	CAD-C3D-C4D	-2.48	124.32	127.01
5	C	2	HEA	CBA-CAA-C2A	-2.40	108.23	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2	HEA	CBA-CAA-C2A	-2.36	108.29	112.53
5	A	1	HEA	CMC-C2C-C1C	-2.35	124.48	128.36
5	A	1	HEA	CMB-C2B-C1B	-2.32	124.53	128.36
5	C	1	HEA	CMB-C2B-C1B	-2.31	124.54	128.36
5	A	2	HEA	C13-C14-C15	-2.30	122.77	127.76
5	C	1	HEA	CMC-C2C-C1C	-2.25	124.65	128.36
3	B	1	DMU	O3-C5-C10	-2.24	105.10	110.02
3	B	2	DMU	C10-O7-C3	-2.21	112.24	118.01
5	A	1	HEA	C13-C14-C15	-2.20	122.98	127.76
5	C	2	HEA	CMB-C2B-C1B	-2.20	124.73	128.36
5	C	2	HEA	C3A-C4A-NA	-2.12	106.94	110.94
5	C	1	HEA	CBA-CAA-C2A	-2.07	108.81	112.53
5	C	1	HEA	C17-C18-C19	-2.02	123.37	127.76
5	C	2	HEA	OMA-CMA-C3A	-2.01	121.05	125.11
5	A	2	HEA	OMA-CMA-C3A	-2.00	121.07	125.11
5	C	1	HEA	C25-C23-C24	2.01	119.57	114.64
3	C	10	DMU	C10-O1-C9	2.03	117.68	113.75
5	C	1	HEA	C26-C15-C16	2.12	118.64	115.41
5	C	2	HEA	C25-C23-C24	2.35	120.42	114.64
5	C	1	HEA	C27-C19-C20	2.36	119.01	115.41
5	C	2	HEA	C27-C19-C20	2.55	119.30	115.41
3	B	1	DMU	O16-C6-C1	2.61	111.34	108.04
5	A	1	HEA	C26-C15-C16	2.62	119.40	115.41
5	A	2	HEA	C27-C19-C20	2.65	119.45	115.41
5	A	2	HEA	C26-C15-C16	2.66	119.47	115.41
5	A	1	HEA	C27-C19-C20	2.66	119.47	115.41
3	A	1005	DMU	O16-C6-C1	2.74	111.50	108.04
3	B	1	DMU	O1-C9-C11	2.74	113.27	106.36
5	C	2	HEA	C26-C15-C16	2.77	119.64	115.41
5	C	2	HEA	CBD-CAD-C3D	3.01	117.92	112.53
3	B	2	DMU	O16-C6-C1	3.02	111.85	108.04
3	A	7	DMU	O16-C6-C1	3.05	111.89	108.04
5	A	2	HEA	CBD-CAD-C3D	3.08	118.05	112.53
3	D	4	DMU	C10-O1-C9	3.41	120.36	113.75

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	1	HEA	ND
5	C	1	HEA	NB
5	C	2	HEA	NB
5	C	2	HEA	NA

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Mol	Chain	Res	Type	Atom
5	C	2	HEA	ND
3	C	9	DMU	C10
5	A	2	HEA	NB
5	A	2	HEA	NA
5	A	2	HEA	ND
5	A	1	HEA	ND
5	A	1	HEA	NB

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	HEA	2	0
3	A	1005	DMU	1	0
5	A	2	HEA	8	0
5	C	1	HEA	1	0
3	C	10	DMU	1	0
5	C	2	HEA	6	0
4	C	3	TRD	1	0
3	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%)	-0.05	28 (5%)	31 24	30, 46, 68, 90	0
1	C	531/535 (99%)	0.30	48 (9%)	12 8	43, 65, 87, 95	0
2	B	256/256 (100%)	-0.27	6 (2%)	64 57	33, 50, 69, 75	1 (0%)
2	D	256/256 (100%)	-0.15	9 (3%)	48 40	42, 56, 79, 88	1 (0%)
All	All	1578/1582 (99%)	0.02	91 (5%)	26 20	30, 54, 80, 95	2 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	THR	6.3
1	C	218	PRO	5.7
1	C	138	MET	5.3
1	C	222	MET	4.7
2	D	99	PRO	4.5
1	C	22	MET	4.4
1	A	22	MET	4.4
1	C	74	LYS	4.2
1	C	20	TRP	4.2
1	C	21	PHE	4.0
1	A	424	MET	3.9
1	C	77	PHE	3.8
2	D	96	HIS	3.5
2	B	56	TRP	3.5
1	A	20	TRP	3.5
1	C	23	SER	3.4
1	A	18	THR	3.4
1	C	71	GLY	3.3
1	A	222	MET	3.2
1	A	423	VAL	3.2
1	A	172	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	259	PHE	3.1
2	D	97	ASN	3.1
2	B	87	ARG	3.1
1	C	171	GLY	3.1
1	C	217	ALA	3.0
2	B	99	PRO	3.0
2	D	87	ARG	3.0
1	C	137	ARG	3.0
1	A	425	SER	3.0
1	C	103	GLY	2.9
1	C	481	ARG	2.8
1	A	223	HIS	2.8
2	B	284	HIS	2.8
1	C	290	ILE	2.8
1	C	426	LEU	2.7
2	B	281	GLN	2.7
1	C	172	TRP	2.6
1	A	420	PHE	2.6
1	C	100	THR	2.6
1	C	413	THR	2.6
1	C	425	SER	2.6
1	C	378	LYS	2.6
1	C	69	GLU	2.6
1	C	107	MET	2.6
1	C	417	VAL	2.6
1	C	219	GLY	2.5
1	A	426	LEU	2.5
1	C	106	MET	2.5
1	C	287	VAL	2.5
1	C	427	GLY	2.5
2	D	100	LEU	2.5
2	D	178	GLN	2.5
2	D	98	SER	2.4
1	A	397	THR	2.4
1	C	73	VAL	2.4
1	A	421	HIS	2.4
1	A	214	ASN	2.4
1	C	81	TRP	2.3
1	A	287	VAL	2.3
1	A	401	LEU	2.3
1	A	427	GLY	2.3
1	C	140	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	263	PHE	2.3
2	B	81	TRP	2.3
1	C	428	ALA	2.3
1	C	416	VAL	2.2
2	D	56	TRP	2.2
1	C	70	SER	2.2
1	C	99	ILE	2.2
1	A	398	GLY	2.2
1	C	446	ARG	2.2
1	C	412	ASP	2.2
1	A	290	ILE	2.1
1	A	428	ALA	2.1
1	A	394	GLY	2.1
1	C	184	GLY	2.1
1	A	220	MET	2.1
1	A	260	GLY	2.1
1	A	221	THR	2.1
1	A	291	VAL	2.1
1	A	417	VAL	2.1
1	A	81	TRP	2.1
1	C	414	TYR	2.1
1	C	75	GLY	2.0
1	C	267	SER	2.0
1	C	173	VAL	2.0
1	C	429	VAL	2.0
2	D	81	TRP	2.0
1	C	398	GLY	2.0
1	A	548	GLU	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	TRD	A	1013	7/13	0.70	0.32	8.54	60,61,61,61	0
3	DMU	A	1005	22/33	0.85	0.25	7.12	56,59,63,63	22
4	TRD	D	14	7/13	0.82	0.44	6.87	41,42,42,43	0
3	DMU	C	10	33/33	0.83	0.33	6.64	52,54,56,57	0
9	HTH	B	286	10/10	0.86	0.44	5.46	62,66,68,68	0
4	TRD	B	4	9/13	0.88	0.34	4.64	73,73,75,76	0
3	DMU	B	3	33/33	0.85	0.27	1.56	95,99,101,101	0
4	TRD	A	3	13/13	0.84	0.28	1.48	61,63,64,64	0
4	TRD	C	3	13/13	0.90	0.23	1.18	68,69,73,73	0
7	MG	A	6	1/1	0.99	0.25	1.10	23,23,23,23	0
3	DMU	C	9	12/33	0.73	0.26	1.05	91,92,92,92	12
5	HEA	A	2	60/60	0.94	0.30	0.78	41,48,58,59	0
4	TRD	A	1009	7/13	0.87	0.17	0.61	62,63,63,64	0
3	DMU	A	7	22/33	0.83	0.20	0.60	51,72,80,80	0
3	DMU	B	1	33/33	0.95	0.14	0.33	39,45,59,61	0
7	MG	C	6	1/1	0.99	0.23	0.30	31,31,31,31	0
5	HEA	C	2	60/60	0.95	0.23	0.08	44,53,63,64	0
5	HEA	C	1	60/60	0.97	0.25	0.04	45,47,54,55	0
5	HEA	A	1	60/60	0.98	0.22	-0.09	31,35,40,41	0
6	CU1	D	3	1/1	1.00	0.15	-0.29	47,47,47,47	0
6	CU1	D	286	1/1	1.00	0.13	-0.57	44,44,44,44	0
6	CU1	B	287	1/1	1.00	0.15	-0.83	37,37,37,37	0
8	CA	A	553	1/1	0.99	0.10	-0.94	34,34,34,34	0
6	CU1	B	288	1/1	1.00	0.13	-1.06	34,34,34,34	0
10	CD	B	9	1/1	0.99	0.06	-2.03	79,79,79,79	1
8	CA	C	7	1/1	0.94	0.09	-2.29	57,57,57,57	0
10	CD	B	8	1/1	1.00	0.08	-2.58	52,52,52,52	0
10	CD	D	287	1/1	0.99	0.07	-2.79	54,54,54,54	0
3	DMU	B	2	33/33	0.78	0.34	-	65,69,86,87	25
3	DMU	D	4	23/33	0.83	0.29	-	88,89,91,91	23
3	DMU	C	5	23/33	0.83	0.26	-	99,100,101,101	23
6	CU1	C	553	1/1	0.98	0.17	-	54,54,54,54	0
10	CD	D	9	1/1	0.86	0.08	-	95,95,95,95	1
3	DMU	D	8	23/33	0.78	0.37	-	88,90,92,92	23
4	TRD	A	552	13/13	0.80	0.31	-	72,73,77,77	0
4	TRD	C	552	13/13	0.66	0.29	-	94,94,95,95	0
3	DMU	B	6	23/33	0.89	0.18	-	81,82,83,83	23
6	CU1	A	5	1/1	0.99	0.21	-	48,48,48,48	0
4	TRD	A	1015	7/13	0.83	0.48	-	72,72,74,74	0

## 6.5 Other polymers

There are no such residues in this entry.