



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2017 – 06:16 PM EDT

PDB ID : 3FYI
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides in the reduced state bound with cyanide
Authors : Qin, L.; Mills, D.A.; Proshlyakov, D.A.; Hiser, C.; Ferguson-Miller, S.
Deposited on : unknown
Resolution : 2.20 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

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) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

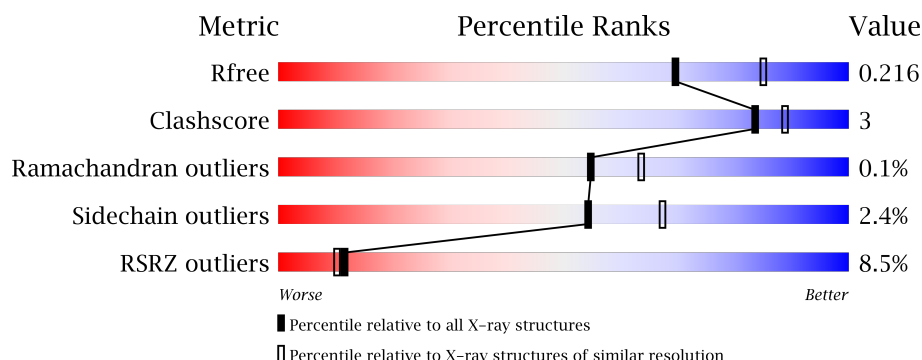
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
1	C	566	<div> <div>14%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
2	B	262	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>•</div> </div> </div>
2	D	262	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </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
10	HTO	B	1	X	-	-	X
3	HEA	A	567	X	-	-	-
3	HEA	A	568	X	-	-	-
3	HEA	C	567	X	-	-	-
3	HEA	C	568	X	-	-	-
5	MG	A	570	-	-	-	X
8	DMU	A	574	-	-	-	X
8	DMU	A	576	-	-	-	X
9	TRD	A	578	-	-	-	X
9	TRD	A	580	-	-	-	X
9	TRD	A	581	-	-	-	X
9	TRD	A	582	-	-	-	X
9	TRD	C	1009	-	-	-	X
9	TRD	C	1010	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	22	0	0
			4212	2822	663	696	31			
1	C	531	Total	C	N	O	S	26	0	0
			4172	2794	656	691	31			

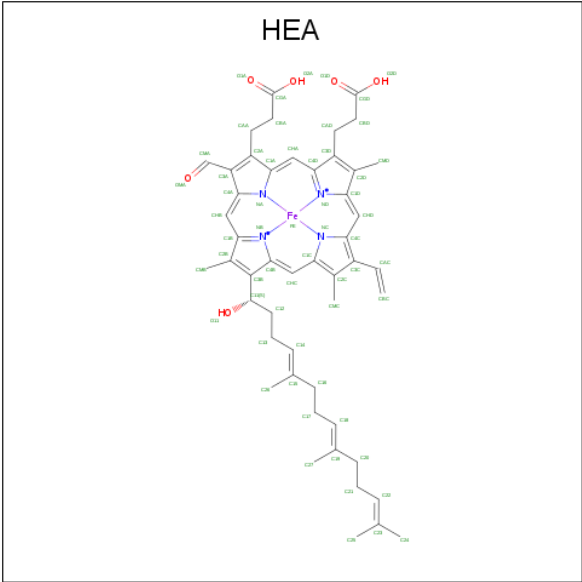
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	4	1	0
			2031	1325	333	367	6			
2	D	256	Total	C	N	O	S	9	1	0
			2031	1325	333	367	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	EXPRESSION TAG	UNP Q03736
B	283	HIS	-	EXPRESSION TAG	UNP Q03736
B	284	HIS	-	EXPRESSION TAG	UNP Q03736
B	285	HIS	-	EXPRESSION TAG	UNP Q03736
B	286	HIS	-	EXPRESSION TAG	UNP Q03736
B	287	HIS	-	EXPRESSION TAG	UNP Q03736
D	282	HIS	-	EXPRESSION TAG	UNP Q03736
D	283	HIS	-	EXPRESSION TAG	UNP Q03736
D	284	HIS	-	EXPRESSION TAG	UNP Q03736
D	285	HIS	-	EXPRESSION TAG	UNP Q03736
D	286	HIS	-	EXPRESSION TAG	UNP Q03736
D	287	HIS	-	EXPRESSION TAG	UNP Q03736

- Molecule 3 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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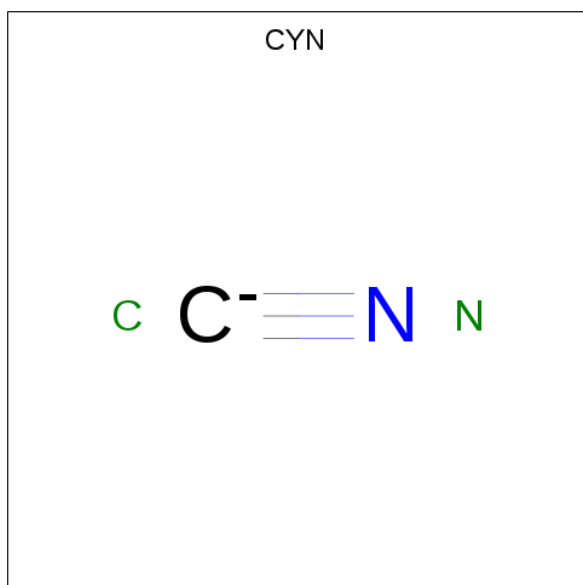
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

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

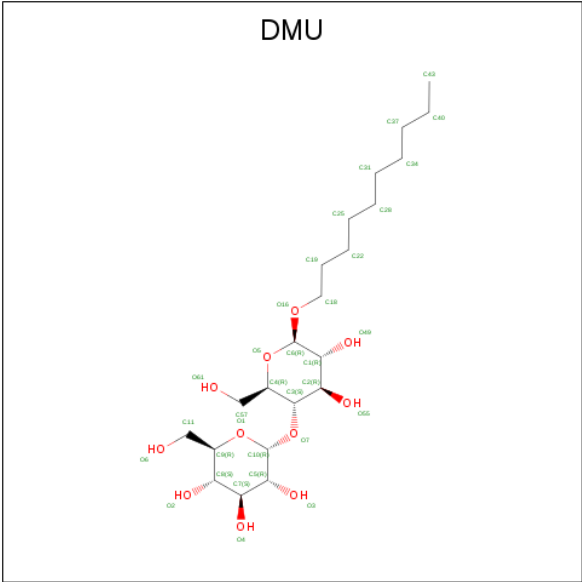
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 is CYANIDE ION (three-letter code: CYN) (formula: CN).



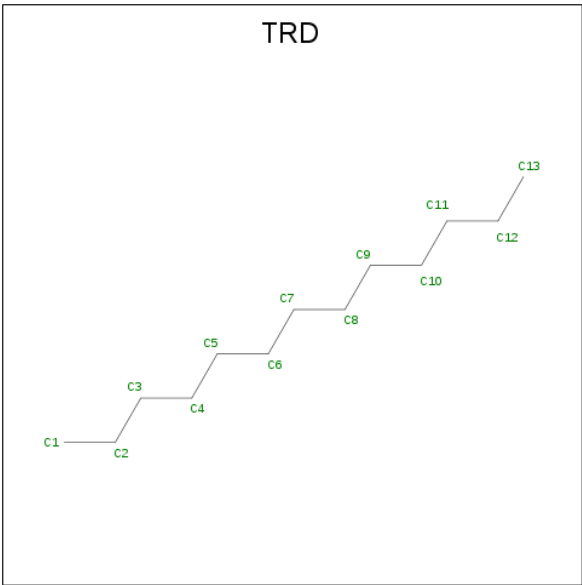
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			2	1	1		
7	C	1	Total	C	N	0	0
			2	1	1		

- Molecule 8 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



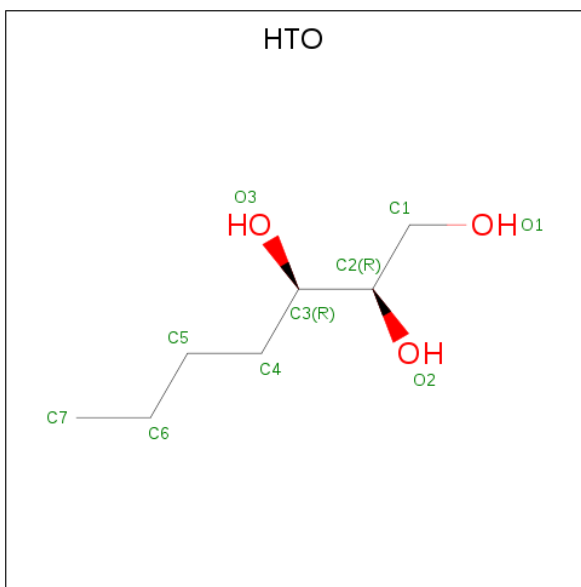
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			33	22	11		
8	A	1	Total	C	O	0	0
			33	22	11		
8	A	1	Total	C	O	0	0
			22	16	6		
8	A	1	Total	C	O	0	0
			33	22	11		
8	B	1	Total	C	O	0	0
			33	22	11		
8	B	1	Total	C	O	0	0
			23	12	11		
8	C	1	Total	C	O	0	0
			23	12	11		
8	C	1	Total	C	O	0	0
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

- Molecule 9 is TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



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

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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

- Molecule 11 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

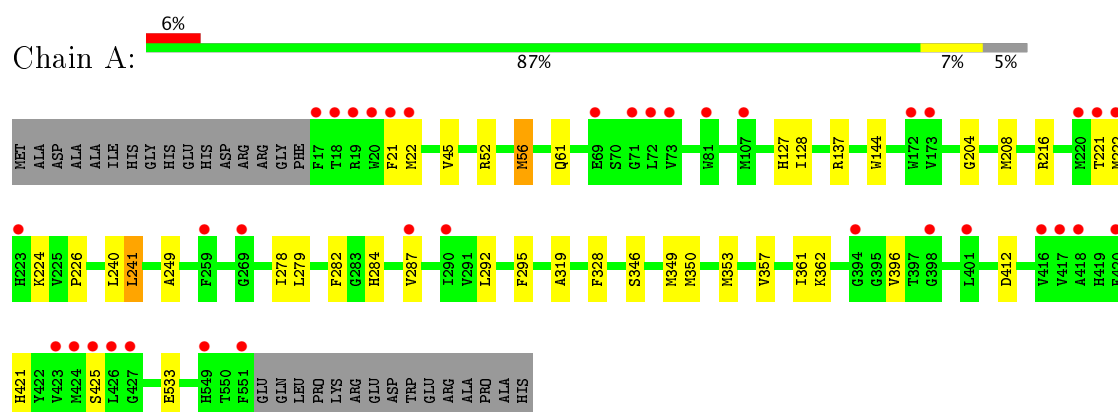
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	126	Total O 126 126	0	0
12	B	133	Total O 133 133	0	0
12	C	102	Total O 102 102	0	0
12	D	109	Total O 109 109	0	0

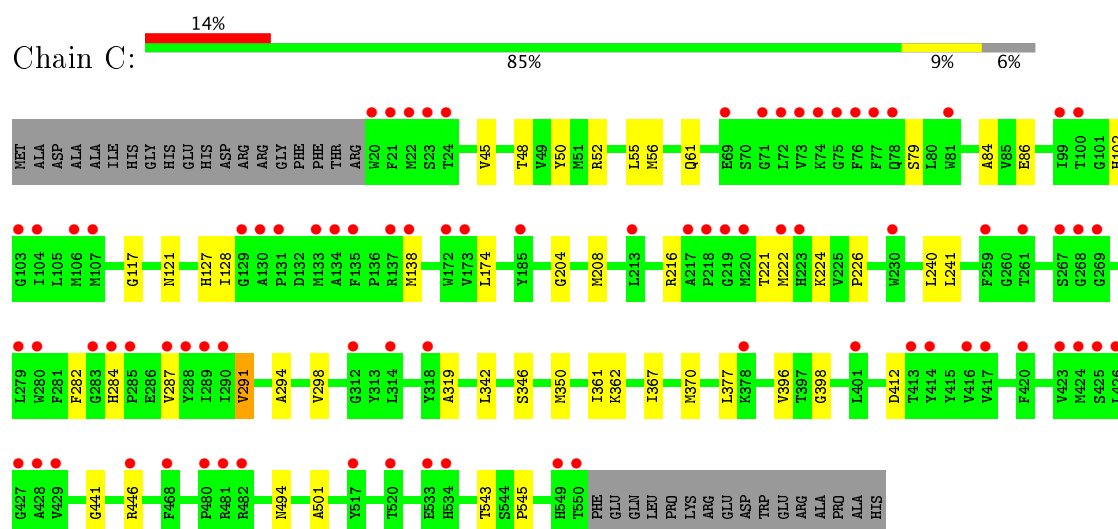
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

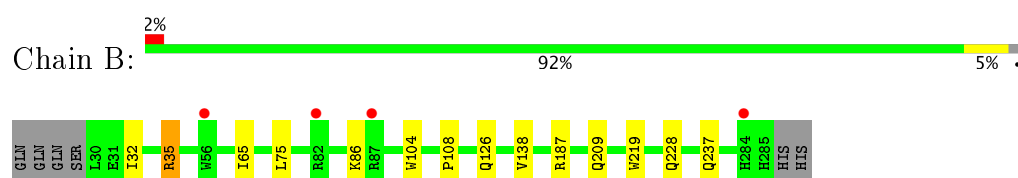
• Molecule 1: Cytochrome c oxidase subunit 1



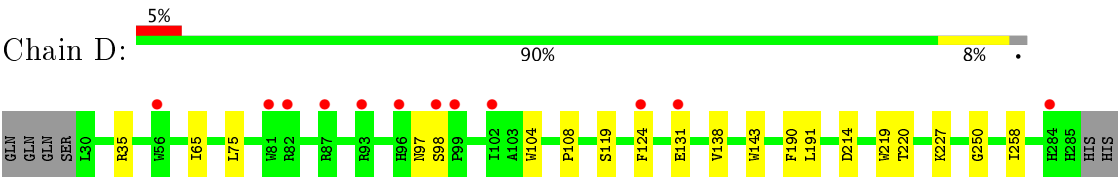
• Molecule 1: Cytochrome c oxidase subunit 1



• 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, α , β , γ	124.34Å 131.88Å 176.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 41.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.2 (41.77-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.219 0.193 , 0.216	Depositor DCC
R_{free} test set	3933 reflections (2.86%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13601	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, HTO, CA, TRD, CD, DMU, CYN, 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	0/4368	0.54	0/5961
1	C	0.46	0/4326	0.51	0/5905
2	B	0.51	0/2096	0.55	0/2869
2	D	0.46	0/2096	0.53	0/2869
All	All	0.50	0/12886	0.53	0/17604

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	4212	0	4134	26	0
1	C	4172	0	4097	29	0
2	B	2031	0	1988	8	0
2	D	2031	0	1988	8	0
3	A	120	0	108	5	0
3	C	120	0	108	8	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	0	0
7	C	2	0	0	0	0
8	A	121	0	157	1	0
8	B	56	0	63	1	0
8	C	56	0	63	2	0
8	D	56	0	63	1	0
9	A	66	0	138	0	0
9	C	42	0	86	2	0
9	D	20	0	41	0	0
10	B	10	0	16	0	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
12	A	126	0	0	0	0
12	B	133	0	0	2	0
12	C	102	0	0	0	0
12	D	109	0	0	0	0
All	All	13601	0	13050	74	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 3.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:GLN:NE2	12:B:389:HOH:O	1.96	0.95
2:B:32:ILE:HG22	2:B:35:ARG:HD3	1.58	0.86
3:C:568:HEA:HBD2	3:C:568:HEA:HMD1	1.61	0.81
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.45	0.81
3:C:567:HEA:HMC1	3:C:567:HEA:HBC1	1.62	0.79
3:A:568:HEA:HBD2	3:A:568:HEA:HMD1	1.69	0.75
1:C:56:MET:HE1	8:C:1005:DMU:H7	1.73	0.69
3:A:567:HEA:HMC1	3:A:567:HEA:HBC1	1.74	0.68
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.29	0.66
1:C:84:ALA:HB1	1:C:86:GLU:OE1	1.95	0.65
1:A:396:VAL:HB	2:B:65:ILE:HB	1.80	0.63
1:C:50:TYR:OH	1:C:79:SER:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:GLY:O	1:C:208:MET:HG2	1.99	0.62
1:C:284:HIS:CD2	1:C:284:HIS:C	2.74	0.60
1:A:56:MET:HE1	8:A:576:DMU:H7	1.84	0.60
1:A:357:VAL:O	1:A:361:ILE:HG12	2.02	0.59
1:C:396:VAL:HB	2:D:65:ILE:HB	1.84	0.59
1:A:221:THR:CG2	1:A:224:LYS:HG2	2.34	0.57
1:A:204:GLY:O	1:A:208:MET:HG2	2.07	0.55
1:C:361:ILE:HD11	2:D:108:PRO:HG2	1.90	0.54
1:A:287:VAL:HB	3:A:568:HEA:HAC	1.90	0.53
3:C:568:HEA:CBD	3:C:568:HEA:HMD1	2.35	0.53
1:C:287:VAL:HB	3:C:568:HEA:HAC	1.91	0.52
1:A:284:HIS:CD2	1:A:284:HIS:C	2.83	0.52
1:A:361:ILE:HD11	2:B:108:PRO:HG2	1.93	0.50
1:C:86:GLU:H	1:C:86:GLU:CD	2.16	0.49
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.93	0.49
1:C:284:HIS:O	1:C:287:VAL:HG22	2.12	0.49
1:C:221:THR:HG22	1:C:224:LYS:HG3	1.94	0.49
2:B:35:ARG:HD2	12:B:343:HOH:O	2.12	0.49
1:C:128:ILE:HB	1:C:216:ARG:HG2	1.95	0.48
1:C:398:GLY:O	3:C:568:HEA:HMB3	2.13	0.48
1:A:221:THR:HG22	1:A:224:LYS:CG	2.43	0.48
1:A:221:THR:HG23	1:A:224:LYS:HG2	1.95	0.48
1:C:367:ILE:HA	1:C:370:MET:HE2	1.95	0.47
1:A:221:THR:HG22	1:A:224:LYS:HG3	1.96	0.47
1:C:48:THR:CG2	1:C:102:HIS:CE1	2.97	0.46
1:A:349:MET:O	1:A:353:MET:HE2	2.15	0.46
3:C:568:HEA:HHC	3:C:568:HEA:H122	1.97	0.46
1:A:533:GLU:CD	1:A:533:GLU:H	2.19	0.46
1:A:292:LEU:O	1:A:295:PHE:HB2	2.16	0.46
1:C:342:LEU:HD21	2:D:124:PHE:CD2	2.50	0.45
1:C:319:ALA:HB3	1:C:362:LYS:HE2	1.99	0.45
1:C:55:LEU:O	1:C:494:ASN:HB3	2.16	0.45
1:C:441:GLY:HA2	1:C:446:ARG:O	2.16	0.45
1:C:52:ARG:HG3	1:C:501:ALA:CB	2.47	0.45
1:A:249:ALA:HB2	1:A:278:ILE:HG22	1.99	0.45
1:A:279:LEU:C	1:A:279:LEU:HD13	2.38	0.45
1:A:346:SER:O	1:A:350:MET:HG2	2.17	0.44
1:A:128:ILE:HB	1:A:216:ARG:HG2	2.00	0.44
1:C:543:THR:HG23	1:C:545:PRO:O	2.18	0.44
2:D:75:LEU:HD13	8:D:1003:DMU:H18	2.00	0.43
1:A:319:ALA:HB3	1:A:362:LYS:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:HIS:HA	1:A:425:SER:HB2	2.00	0.43
1:C:127:HIS:HB3	1:C:226:PRO:HG2	2.01	0.43
1:C:377:LEU:HD13	9:C:1010:TRD:H31	2.00	0.43
1:C:291:VAL:HB	3:C:568:HEA:HBC2	2.00	0.43
1:C:367:ILE:HA	1:C:370:MET:CE	2.49	0.43
2:B:75:LEU:HD13	8:B:288:DMU:H18	2.01	0.42
2:D:143:TRP:CH2	2:D:258:ILE:HG22	2.53	0.42
2:D:220:THR:O	2:D:250:GLY:HA3	2.20	0.42
1:A:241:LEU:HB3	1:A:328:PHE:CZ	2.55	0.42
1:A:45:VAL:HG21	3:A:567:HEA:H171	2.01	0.42
1:A:221:THR:CG2	1:A:224:LYS:CG	2.97	0.42
1:C:346:SER:O	1:C:350:MET:HG2	2.20	0.42
2:D:190:PHE:O	2:D:191:LEU:HB2	2.20	0.42
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.55	0.42
1:C:294:ALA:O	1:C:298:VAL:HG23	2.20	0.41
2:B:209:GLN:HG2	2:B:237:GLN:HG2	2.02	0.41
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.56	0.41
1:C:117:GLY:O	1:C:121:ASN:HB2	2.20	0.41
1:C:45:VAL:HG21	3:C:567:HEA:H171	2.02	0.41
8:C:1005:DMU:H9	9:C:1006:TRD:H81	2.04	0.40
3:A:568:HEA:H122	3:A:568:HEA:HHC	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/566 (94%)	523 (98%)	10 (2%)	0	100	100
1	C	529/566 (94%)	524 (99%)	5 (1%)	0	100	100
2	B	255/262 (97%)	249 (98%)	6 (2%)	0	100	100
2	D	255/262 (97%)	249 (98%)	5 (2%)	1 (0%)	38	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1572/1656 (95%)	1545 (98%)	26 (2%)	1 (0%)	55 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	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	435/459 (95%)	425 (98%)	10 (2%)	56 69
1	C	431/459 (94%)	422 (98%)	9 (2%)	59 72
2	B	216/221 (98%)	211 (98%)	5 (2%)	56 69
2	D	216/221 (98%)	209 (97%)	7 (3%)	44 56
All	All	1298/1360 (95%)	1267 (98%)	31 (2%)	54 67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	52	ARG
1	A	56	MET
1	A	61	GLN
1	A	137	ARG
1	A	222	MET
1	A	240	LEU
1	A	241	LEU
1	A	282	PHE
1	A	412	ASP
2	B	35	ARG
2	B	86	LYS
2	B	104	TRP
2	B	126	GLN

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Mol	Chain	Res	Type
2	B	187	ARG
1	C	61	GLN
1	C	138	MET
1	C	174	LEU
1	C	222	MET
1	C	240	LEU
1	C	241	LEU
1	C	282	PHE
1	C	291	VAL
1	C	412	ASP
2	D	35	ARG
2	D	98	SER
2	D	104	TRP
2	D	119	SER
2	D	131	GLU
2	D	214	ASP
2	D	227	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	534	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 14 are monoatomic - leaving 29 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
3	HEA	A	567	1	44,67,67	1.78	8 (18%)	37,103,103	1.34	7 (18%)
3	HEA	A	568	1	44,67,67	1.31	6 (13%)	37,103,103	1.81	11 (29%)
7	CYN	A	572	4	0,1,1	0.00	-	0,0,0	0.00	-
8	DMU	A	573	-	34,34,34	0.50	0	45,45,45	0.97	3 (6%)
8	DMU	A	574	-	34,34,34	0.58	1 (2%)	45,45,45	0.85	2 (4%)
8	DMU	A	575	-	22,22,34	0.59	1 (4%)	27,27,45	0.85	1 (3%)
8	DMU	A	576	-	34,34,34	0.60	0	45,45,45	0.76	0
9	TRD	A	577	-	12,12,12	0.25	0	11,11,11	0.48	0
9	TRD	A	578	-	12,12,12	0.27	0	11,11,11	0.51	0
9	TRD	A	579	-	6,6,12	0.26	0	5,5,11	0.35	0
9	TRD	A	580	-	6,6,12	0.24	0	5,5,11	0.38	0
9	TRD	A	581	-	12,12,12	0.26	0	11,11,11	0.53	0
9	TRD	A	582	-	12,12,12	0.28	0	11,11,11	0.51	0
10	HTO	B	1	-	9,9,9	0.34	0	9,10,10	0.96	1 (11%)
8	DMU	B	11	-	24,24,34	0.51	0	35,35,45	0.74	0
8	DMU	B	288	-	34,34,34	0.54	0	45,45,45	0.74	0
9	TRD	C	1001	-	12,12,12	0.25	0	11,11,11	0.51	0
8	DMU	C	1002	-	24,24,34	0.53	0	35,35,45	0.68	0
8	DMU	C	1005	-	34,34,34	0.60	1 (2%)	45,45,45	0.89	0
9	TRD	C	1006	-	12,12,12	0.27	0	11,11,11	0.49	0
9	TRD	C	1009	-	6,6,12	0.26	0	5,5,11	0.34	0
9	TRD	C	1010	-	8,8,12	0.27	0	7,7,11	0.39	0
3	HEA	C	567	1	44,67,67	1.66	8 (18%)	37,103,103	1.34	7 (18%)
3	HEA	C	568	1	44,67,67	1.32	4 (9%)	37,103,103	1.83	12 (32%)
7	CYN	C	572	4	0,1,1	0.00	-	0,0,0	0.00	-
8	DMU	D	1003	-	34,34,34	0.54	0	45,45,45	0.64	0
9	TRD	D	1007	-	12,12,12	0.23	0	11,11,11	0.58	0
9	TRD	D	1008	-	6,6,12	0.25	0	5,5,11	0.40	0
8	DMU	D	1011	-	24,24,34	0.52	0	35,35,45	0.88	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
3	HEA	A	567	1	2/2/7/16	0/24/76/76	0/0/8/8
3	HEA	A	568	1	2/2/7/16	0/24/76/76	0/0/8/8
7	CYN	A	572	4	-	0/0/0/0	0/0/0/0
8	DMU	A	573	-	-	0/19/59/59	0/2/2/2
8	DMU	A	574	-	-	0/19/59/59	0/2/2/2
8	DMU	A	575	-	-	0/13/33/59	0/1/1/2
8	DMU	A	576	-	-	0/19/59/59	0/2/2/2
9	TRD	A	577	-	-	0/10/10/10	0/0/0/0
9	TRD	A	578	-	-	0/10/10/10	0/0/0/0
9	TRD	A	579	-	-	0/4/4/10	0/0/0/0
9	TRD	A	580	-	-	0/4/4/10	0/0/0/0
9	TRD	A	581	-	-	0/10/10/10	0/0/0/0
9	TRD	A	582	-	-	0/10/10/10	0/0/0/0
10	HTO	B	1	-	1/1/2/2	0/10/10/10	0/0/0/0
8	DMU	B	11	-	-	0/8/48/59	0/2/2/2
8	DMU	B	288	-	-	0/19/59/59	0/2/2/2
9	TRD	C	1001	-	-	0/10/10/10	0/0/0/0
8	DMU	C	1002	-	-	0/8/48/59	0/2/2/2
8	DMU	C	1005	-	-	0/19/59/59	0/2/2/2
9	TRD	C	1006	-	-	0/10/10/10	0/0/0/0
9	TRD	C	1009	-	-	0/4/4/10	0/0/0/0
9	TRD	C	1010	-	-	0/6/6/10	0/0/0/0
3	HEA	C	567	1	3/3/7/16	0/24/76/76	0/0/8/8
3	HEA	C	568	1	2/2/7/16	0/24/76/76	0/0/8/8
7	CYN	C	572	4	-	0/0/0/0	0/0/0/0
8	DMU	D	1003	-	-	0/19/59/59	0/2/2/2
9	TRD	D	1007	-	-	0/10/10/10	0/0/0/0
9	TRD	D	1008	-	-	0/4/4/10	0/0/0/0
8	DMU	D	1011	-	-	0/8/48/59	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	567	HEA	C3A-C2A	-5.87	1.32	1.40
3	C	567	HEA	C3A-C2A	-5.19	1.33	1.40
3	C	567	HEA	C3C-C2C	-4.64	1.34	1.40
3	A	567	HEA	C3C-C2C	-4.41	1.34	1.40
3	C	568	HEA	C3A-C2A	-3.94	1.35	1.40
3	A	568	HEA	C3A-C2A	-3.91	1.35	1.40
3	C	568	HEA	C3C-C2C	-3.34	1.35	1.40
3	A	568	HEA	C3C-C2C	-3.21	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	567	HEA	C3B-C2B	-2.30	1.33	1.41
3	C	567	HEA	C3B-C2B	-2.26	1.33	1.41
3	C	567	HEA	C4B-NB	2.00	1.39	1.36
3	C	567	HEA	C1D-ND	2.03	1.39	1.36
3	C	567	HEA	C3A-CMA	2.04	1.51	1.46
8	C	1005	DMU	O16-C6	2.04	1.43	1.40
8	A	574	DMU	O16-C6	2.07	1.43	1.40
3	A	568	HEA	C4D-ND	2.10	1.40	1.36
3	C	567	HEA	C4A-NA	2.12	1.39	1.36
8	A	575	DMU	O16-C6	2.12	1.43	1.40
3	A	568	HEA	C4B-NB	2.19	1.39	1.36
3	A	567	HEA	CAD-C3D	2.21	1.55	1.52
3	A	568	HEA	CAD-C3D	2.24	1.55	1.52
3	A	567	HEA	C1D-ND	2.27	1.39	1.36
3	A	567	HEA	C4B-NB	2.31	1.39	1.36
3	A	568	HEA	C3C-CAC	2.41	1.52	1.47
3	C	568	HEA	C3C-CAC	2.51	1.52	1.47
3	C	568	HEA	C4B-NB	2.76	1.40	1.36
3	A	567	HEA	C1A-NA	3.39	1.40	1.36
3	C	567	HEA	C3C-CAC	3.47	1.54	1.47
3	A	567	HEA	C3C-CAC	3.77	1.55	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	568	HEA	CBA-CAA-C2A	-3.79	105.24	112.47
3	C	568	HEA	C3C-C4C-NC	-3.60	104.56	109.21
3	A	568	HEA	C3C-C4C-NC	-3.60	104.56	109.21
3	C	568	HEA	CBA-CAA-C2A	-3.44	105.91	112.47
3	C	568	HEA	CMC-C2C-C1C	-3.28	123.42	128.46
3	A	568	HEA	CMC-C2C-C1C	-3.25	123.47	128.46
3	C	568	HEA	C17-C18-C19	-2.93	120.32	127.68
3	C	568	HEA	C3A-C4A-NA	-2.88	105.50	110.94
3	A	568	HEA	C3A-C4A-NA	-2.84	105.58	110.94
3	C	567	HEA	CMC-C2C-C1C	-2.71	124.29	128.46
3	A	567	HEA	C13-C12-C11	-2.64	110.47	114.46
3	A	567	HEA	C17-C18-C19	-2.57	121.23	127.68
8	A	573	DMU	C10-O7-C3	-2.56	111.77	118.00
3	A	567	HEA	CMC-C2C-C1C	-2.43	124.73	128.46
3	A	568	HEA	OMA-CMA-C3A	-2.34	119.71	125.08
3	A	568	HEA	C17-C18-C19	-2.33	121.82	127.68
10	B	1	HTO	C5-C4-C3	-2.30	110.35	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	568	HEA	CMB-C2B-C1B	-2.26	124.99	128.46
3	C	567	HEA	CAD-CBD-CGD	-2.24	108.84	112.66
3	C	567	HEA	CMB-C2B-C1B	-2.21	125.06	128.46
3	C	568	HEA	OMA-CMA-C3A	-2.20	120.02	125.08
8	A	574	DMU	C10-O7-C3	-2.20	112.64	118.00
3	A	567	HEA	CMB-C2B-C1B	-2.15	125.16	128.46
8	A	573	DMU	C7-C8-C9	-2.05	106.60	110.22
3	C	567	HEA	C13-C12-C11	-2.02	111.41	114.46
3	C	567	HEA	C4B-C3B-C2B	2.03	108.28	106.87
3	C	567	HEA	C27-C19-C20	2.03	118.81	115.29
3	A	568	HEA	CMC-C2C-C3C	2.04	128.68	124.89
3	A	568	HEA	C27-C19-C20	2.07	118.87	115.29
3	C	567	HEA	C25-C23-C24	2.08	119.45	114.60
3	A	567	HEA	C27-C19-C20	2.21	119.12	115.29
3	A	567	HEA	C4B-C3B-C2B	2.22	108.42	106.87
8	A	573	DMU	O2-C8-C9	2.25	114.95	109.28
3	C	568	HEA	C27-C19-C20	2.25	119.19	115.29
3	C	568	HEA	C25-C23-C24	2.28	119.92	114.60
3	C	568	HEA	CBD-CAD-C3D	2.42	117.12	112.48
3	C	568	HEA	C26-C15-C16	2.63	119.85	115.29
8	A	575	DMU	O16-C6-C1	2.71	112.66	108.23
3	A	567	HEA	C26-C15-C16	2.79	120.14	115.29
8	A	574	DMU	O16-C6-C1	2.90	112.97	108.23
3	A	568	HEA	C1B-C2B-C3B	2.94	109.04	107.00
3	A	568	HEA	C26-C15-C16	2.96	120.43	115.29
3	A	568	HEA	CBD-CAD-C3D	3.02	118.27	112.48
3	C	568	HEA	C1B-C2B-C3B	3.77	109.62	107.00

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	567	HEA	ND
3	A	567	HEA	NB
3	C	567	HEA	ND
3	C	567	HEA	NA
3	C	567	HEA	NB
10	B	1	HTO	C2
3	C	568	HEA	ND
3	C	568	HEA	NB
3	A	568	HEA	ND
3	A	568	HEA	NB

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	567	HEA	2	0
3	A	568	HEA	3	0
8	A	576	DMU	1	0
8	B	288	DMU	1	0
8	C	1005	DMU	2	0
9	C	1006	TRD	1	0
9	C	1010	TRD	1	0
3	C	567	HEA	2	0
3	C	568	HEA	6	0
8	D	1003	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	535/566 (94%)	-0.00	36 (6%) 19 17	23, 34, 57, 72	5 (0%)
1	C	531/566 (93%)	0.64	82 (15%) 2 2	29, 51, 76, 95	5 (0%)
2	B	256/262 (97%)	-0.37	4 (1%) 72 70	22, 37, 55, 60	1 (0%)
2	D	256/262 (97%)	-0.17	12 (4%) 32 31	29, 42, 62, 71	2 (0%)
All	All	1578/1656 (95%)	0.13	134 (8%) 11 10	22, 41, 68, 95	13 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	9.1
1	A	20	TRP	6.6
1	C	222	MET	6.0
2	B	56	TRP	5.2
1	C	22	MET	5.1
1	C	259	PHE	4.7
1	A	22	MET	4.6
1	A	81	TRP	4.5
2	D	96	HIS	4.5
1	C	76	PHE	4.5
1	C	77	PHE	4.5
1	C	287	VAL	4.4
1	C	172	TRP	4.2
1	C	268	GLY	4.2
1	C	21	PHE	4.1
1	C	75	GLY	4.1
2	D	81	TRP	4.0
1	C	520	THR	3.9
1	A	72	LEU	3.9
1	C	218	PRO	3.9
1	C	217	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	533	GLU	3.8
1	C	73	VAL	3.7
1	C	81	TRP	3.7
1	C	318	TYR	3.7
1	C	23	SER	3.6
1	C	549	HIS	3.6
1	C	423	VAL	3.6
2	D	87	ARG	3.6
1	A	17	PHE	3.6
1	C	314	LEU	3.6
1	A	287	VAL	3.5
1	A	420	PHE	3.5
1	C	417	VAL	3.5
1	C	416	VAL	3.5
1	A	424	MET	3.4
1	C	71	GLY	3.4
1	C	223	HIS	3.4
1	A	222	MET	3.3
1	A	423	VAL	3.2
1	A	172	TRP	3.2
1	C	426	LEU	3.2
1	C	267	SER	3.2
1	C	24	THR	3.2
1	C	69	GLU	3.1
1	C	424	MET	3.1
1	C	517	TYR	3.1
1	A	71	GLY	3.0
1	A	21	PHE	3.0
1	C	420	PHE	3.0
1	C	220	MET	3.0
2	D	102	ILE	2.9
1	C	78	GLN	2.9
1	C	283	GLY	2.9
1	C	414	TYR	2.9
1	C	100	THR	2.9
1	A	418	ALA	2.9
1	C	173	VAL	2.8
1	A	290	ILE	2.8
1	C	107	MET	2.8
1	C	289	ILE	2.8
1	C	290	ILE	2.8
1	A	401	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	223	HIS	2.7
1	C	534	HIS	2.7
1	A	173	VAL	2.7
2	D	284	HIS	2.7
1	A	259	PHE	2.7
1	A	417	VAL	2.7
2	D	99	PRO	2.7
1	C	550	THR	2.7
1	C	103	GLY	2.7
2	B	87	ARG	2.7
2	D	56	TRP	2.6
1	C	481	ARG	2.6
1	C	138	MET	2.6
1	A	398	GLY	2.6
1	C	135	PHE	2.6
1	A	107	MET	2.6
1	C	129	GLY	2.6
1	A	69	GLU	2.6
1	C	74	LYS	2.6
1	A	19	ARG	2.5
2	D	98	SER	2.5
1	C	480	PRO	2.5
1	A	220	MET	2.5
1	C	413	THR	2.5
1	C	185	TYR	2.5
1	C	131	PRO	2.5
2	D	124	PHE	2.5
1	C	288	TYR	2.5
1	C	378	LYS	2.5
1	C	134	ALA	2.4
1	A	221	THR	2.4
1	C	261	THR	2.4
1	C	72	LEU	2.4
2	B	284	HIS	2.4
1	C	99	ILE	2.4
1	C	280	TRP	2.4
1	A	426	LEU	2.4
1	C	279	LEU	2.4
1	C	213	LEU	2.4
1	C	427	GLY	2.3
1	A	549	HIS	2.3
2	B	82	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	82	ARG	2.2
2	D	131	GLU	2.2
1	A	269	GLY	2.2
1	A	73	VAL	2.2
1	C	482	ARG	2.2
1	C	285	PRO	2.2
1	A	425	SER	2.2
1	C	137	ARG	2.2
1	C	401	LEU	2.2
1	A	427	GLY	2.2
1	A	416	VAL	2.1
1	C	312	GLY	2.1
1	C	104	ILE	2.1
1	C	446	ARG	2.1
1	C	130	ALA	2.1
1	A	551	PHE	2.1
1	C	269	GLY	2.1
1	A	18	THR	2.1
1	C	428	ALA	2.1
1	C	219	GLY	2.1
1	C	468	PHE	2.0
1	C	133	MET	2.0
1	A	394	GLY	2.0
1	C	284	HIS	2.0
1	C	429	VAL	2.0
1	C	230	TRP	2.0
1	C	106	MET	2.0
1	C	425	SER	2.0
2	D	93	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	DMU	A	576	33/33	0.79	0.24	9.40	41,50,51,52	33
9	TRD	C	1009	7/13	0.76	0.21	7.90	64,65,65,65	0
9	TRD	A	581	13/13	0.64	0.20	6.24	53,60,67,68	0
8	DMU	A	574	33/33	0.89	0.20	5.15	66,72,74,75	0
10	HTO	B	1	10/10	0.82	0.36	4.84	54,57,58,59	0
9	TRD	A	582	13/13	0.75	0.20	4.60	63,66,67,68	0
5	MG	A	570	1/1	0.99	0.26	2.42	17,17,17,17	0
9	TRD	C	1010	9/13	0.64	0.22	2.23	68,69,70,70	0
9	TRD	A	580	7/13	0.81	0.17	2.09	59,59,60,60	0
9	TRD	A	578	13/13	0.90	0.25	2.08	43,45,48,50	0
8	DMU	C	1005	33/33	0.84	0.16	1.59	59,61,62,63	33
9	TRD	A	579	7/13	0.77	0.22	1.54	59,59,60,60	0
9	TRD	D	1007	13/13	0.88	0.23	1.53	51,53,56,57	0
8	DMU	B	288	33/33	0.86	0.24	1.50	77,82,86,86	0
5	MG	C	570	1/1	0.97	0.24	1.30	20,20,20,20	0
9	TRD	D	1008	7/13	0.85	0.16	1.17	61,62,62,63	0
6	CA	A	571	1/1	1.00	0.11	1.13	27,27,27,27	0
8	DMU	D	1003	33/33	0.80	0.28	1.09	93,99,103,103	0
9	TRD	C	1001	13/13	0.56	0.23	0.84	78,79,79,79	0
8	DMU	A	575	22/33	0.80	0.18	0.64	41,61,68,70	0
3	HEA	A	568	60/60	0.96	0.23	0.60	26,31,46,47	0
7	CYN	A	572	2/2	0.99	0.25	0.49	31,31,31,32	0
3	HEA	A	567	60/60	0.98	0.20	0.22	20,23,29,30	0
3	HEA	C	567	60/60	0.96	0.22	0.20	30,33,45,46	0
3	HEA	C	568	60/60	0.95	0.21	0.13	30,37,49,50	0
4	CU1	B	4	1/1	1.00	0.13	0.01	25,25,25,25	0
8	DMU	B	11	23/33	0.82	0.16	-0.01	72,73,75,75	23
8	DMU	A	573	33/33	0.96	0.09	-0.07	24,35,51,53	0
4	CU1	D	4	1/1	1.00	0.12	-0.12	33,33,33,33	0
4	CU1	D	3	1/1	1.00	0.13	-0.40	33,33,33,33	0
7	CYN	C	572	2/2	0.98	0.22	-0.63	36,36,36,37	0
4	CU1	B	3	1/1	1.00	0.12	-1.02	25,25,25,25	0
8	DMU	D	1011	23/33	0.83	0.16	-1.11	68,69,70,70	23
11	CD	D	8	1/1	0.99	0.07	-1.43	40,40,40,40	0
11	CD	B	9	1/1	0.99	0.10	-1.59	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CD	B	8	1/1	0.99	0.07	-1.74	40,40,40,40	0
6	CA	C	571	1/1	0.98	0.04	-2.29	40,40,40,40	0
8	DMU	C	1002	23/33	0.80	0.23	-	97,98,99,99	23
11	CD	D	9	1/1	0.92	0.14	-	45,45,45,45	1
4	CU1	A	569	1/1	1.00	0.16	-	35,35,35,35	0
9	TRD	C	1006	13/13	0.75	0.25	-	72,74,76,76	0
4	CU1	C	569	1/1	0.98	0.14	-	42,42,42,42	0
9	TRD	A	577	13/13	0.74	0.24	-	66,67,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.