



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:09 PM GMT

PDB ID : 1E6Y  
Title : Methyl-coenzyme M reductase from Methanosarcina barkeri  
Authors : Grabarse, W.; Ermler, U.  
Deposited on : 2000-08-23  
Resolution : 1.60 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

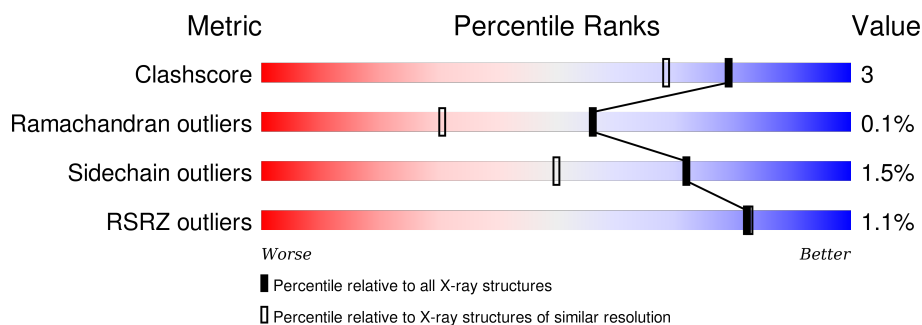
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	569	<div> <div></div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	D	569	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
2	B	433	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
2	E	433	<div> <div></div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
3	C	247	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
3	F	247	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F43	A	2570	X	-	-	-
4	F43	D	5570	X	-	-	-
5	TP7	A	2571	X	-	-	-
5	TP7	D	5571	X	-	-	-
6	COM	A	2572	-	-	-	X
6	COM	D	5572	-	-	-	X
7	GOL	A	2573	-	-	-	X
7	GOL	A	2574	-	-	-	X
7	GOL	D	5573	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21340 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 METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	4	0
			4346	2735	737	846	28			
1	D	568	Total	C	N	O	S	0	3	0
			4348	2738	740	842	28			

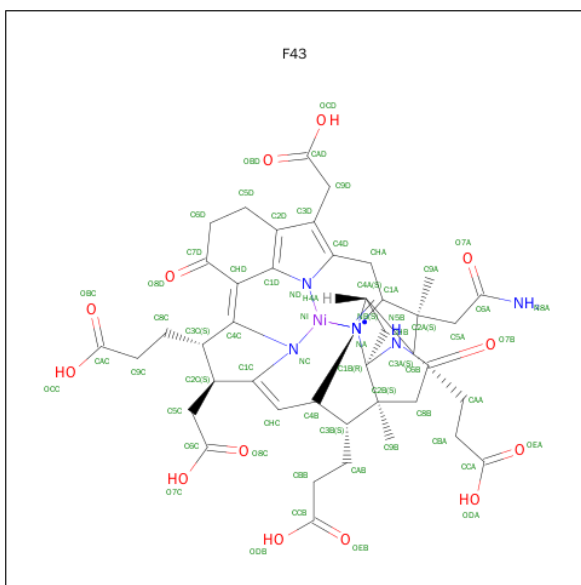
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	4	0
			3176	1987	549	621	19			
2	E	433	Total	C	N	O	S	0	1	0
			3178	1990	550	620	18			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA.

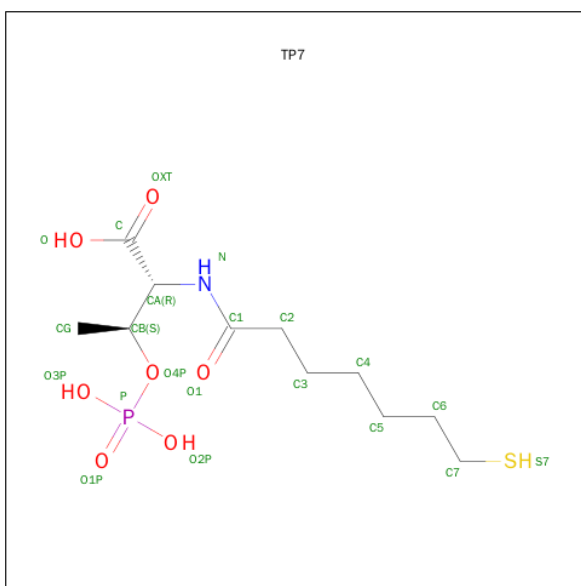
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	0	0
			1947	1202	359	375	11			
3	F	247	Total	C	N	O	S	0	1	0
			1950	1205	359	375	11			

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: C<sub>42</sub>H<sub>49</sub>N<sub>6</sub>NiO<sub>13</sub>).



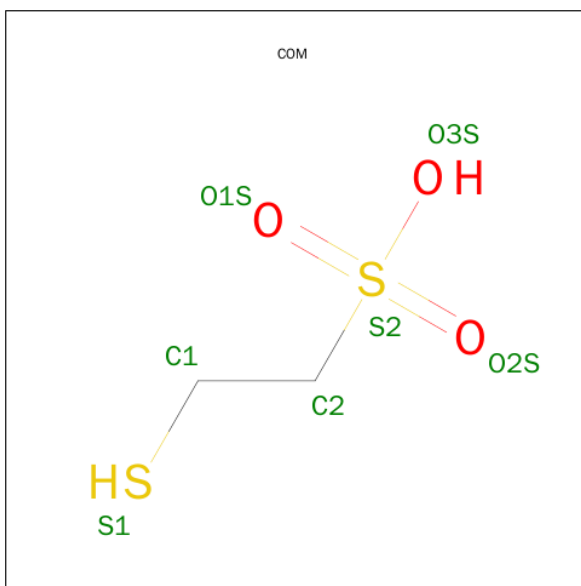
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
4	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

- Molecule 5 is COENZYME B (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).



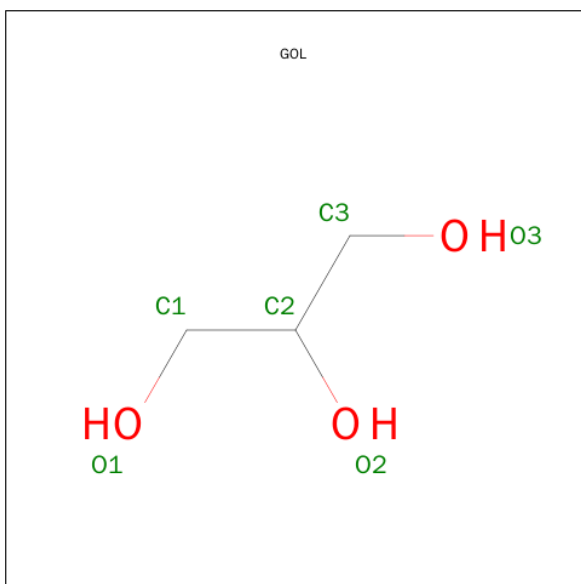
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
5	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			7	2	3	2		
6	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

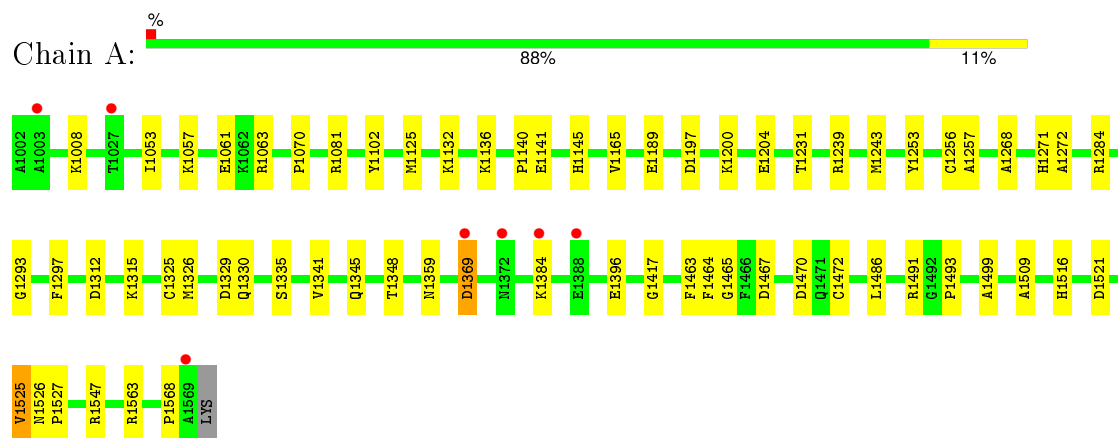
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	489	Total	O	0	0
			489	489		
8	B	340	Total	O	0	2
			342	342		
8	C	241	Total	O	0	0
			241	241		
8	D	522	Total	O	0	0
			522	522		
8	E	339	Total	O	0	0
			339	339		
8	F	264	Total	O	0	0
			264	264		

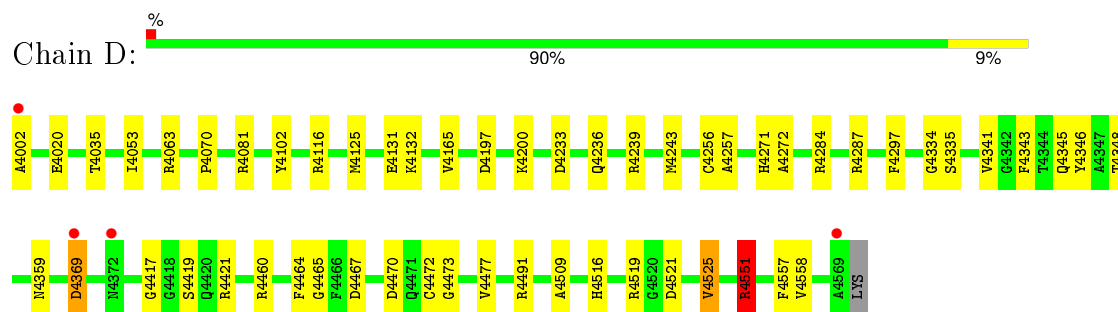
### 3 Residue-property plots [i](#)

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.

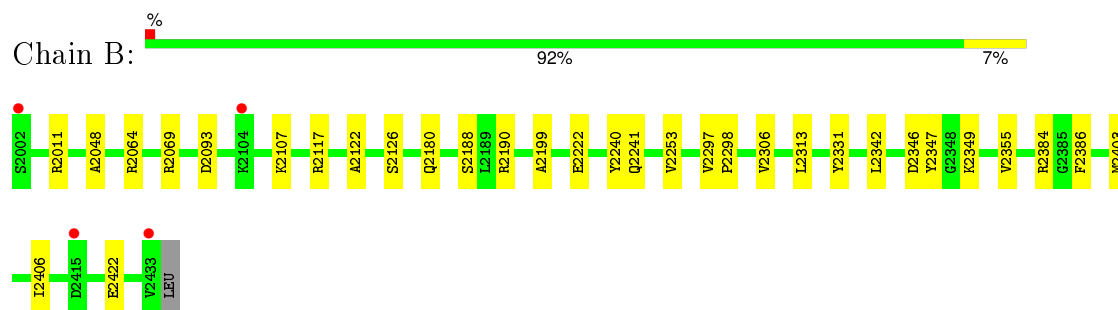
#### • Molecule 1: METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA



#### • Molecule 1: METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA

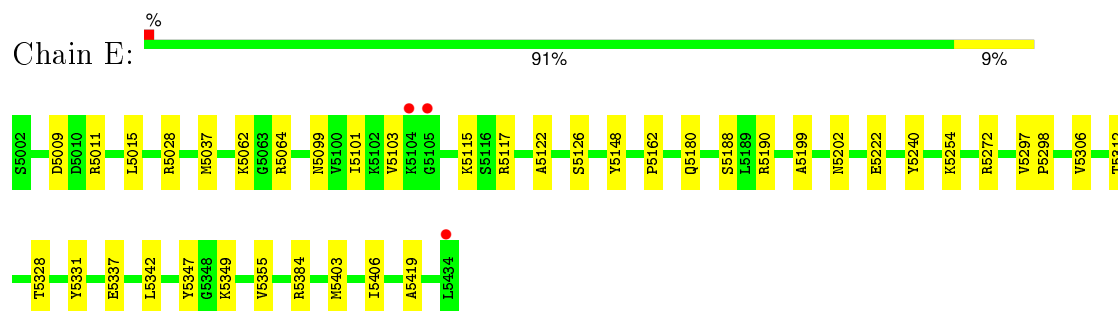


#### • Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

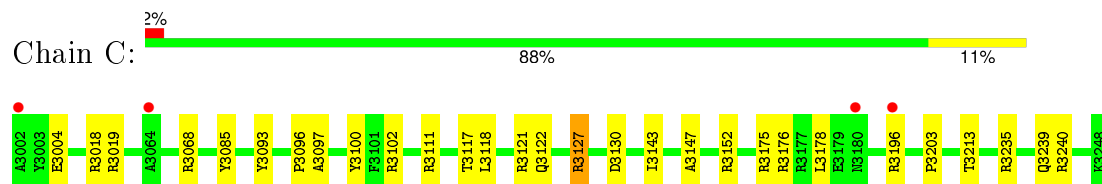


#### • Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

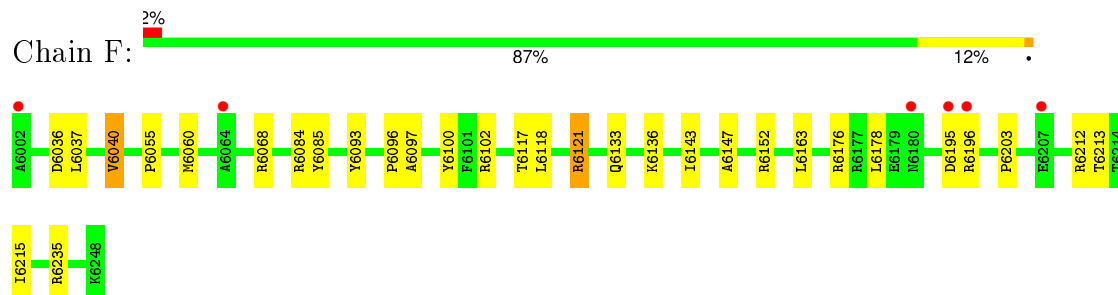




• Molecule 3: METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA



• Molecule 3: METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.68Å 153.10Å 153.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 22.25 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-1.60) 89.2 (22.25-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 1.60Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.160 , 0.179 0.167 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 52.8	EDS
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 326429 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	21340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.2047e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AGM, SMC, F43, TP7, OCS, GL3, COM, MHS

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	0.31	0/4423	0.68	9/5988 (0.2%)
1	D	0.64	6/4418 (0.1%)	1.95	26/5979 (0.4%)
2	B	0.29	0/3244	0.61	8/4390 (0.2%)
2	E	0.30	0/3231	0.65	8/4372 (0.2%)
3	C	0.31	0/1976	0.85	17/2666 (0.6%)
3	F	0.32	0/1983	1.85	15/2676 (0.6%)
All	All	0.41	6/19275 (0.0%)	1.24	83/26071 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	E	0	3
3	C	0	1
3	F	0	1
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4551[A]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[B]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[A]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[B]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[A]	ARG	CG-CD	-8.02	1.31	1.51
1	D	4551[B]	ARG	CG-CD	-8.02	1.31	1.51

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4551[A]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
1	D	4551[B]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
3	F	6040[A]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
3	F	6040[B]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
1	D	4551[A]	ARG	NE-CZ-NH2	-44.85	97.87	120.30
1	D	4551[B]	ARG	NE-CZ-NH2	-44.85	97.87	120.30
1	A	1396[A]	GLU	OE1-CD-OE2	-20.42	98.79	123.30
1	A	1396[B]	GLU	OE1-CD-OE2	-20.42	98.79	123.30
1	D	4551[A]	ARG	NE-CZ-NH1	-20.09	110.25	120.30
1	D	4551[B]	ARG	NE-CZ-NH1	-20.09	110.25	120.30
3	F	6235	ARG	NE-CZ-NH1	19.09	129.84	120.30
1	D	4551[A]	ARG	CG-CD-NE	19.04	151.78	111.80
1	D	4551[B]	ARG	CG-CD-NE	19.04	151.78	111.80
3	F	6235	ARG	NE-CZ-NH2	-14.99	112.80	120.30
1	D	4421	ARG	NE-CZ-NH2	14.53	127.57	120.30
2	E	5384	ARG	NE-CZ-NH1	-11.98	114.31	120.30
2	E	5384	ARG	NE-CZ-NH2	11.51	126.05	120.30
1	D	4551[A]	ARG	CB-CG-CD	10.96	140.11	111.60
1	D	4551[B]	ARG	CB-CG-CD	10.96	140.11	111.60
2	E	5190	ARG	NE-CZ-NH1	-10.65	114.97	120.30
3	C	3121	ARG	NE-CZ-NH1	10.58	125.59	120.30
3	C	3121	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	1547	ARG	CD-NE-CZ	10.23	137.93	123.60
3	F	6235	ARG	CD-NE-CZ	10.13	137.78	123.60
2	B	2384	ARG	NE-CZ-NH1	-9.99	115.31	120.30
2	B	2190	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	D	4460	ARG	NE-CZ-NH2	9.11	124.86	120.30
2	B	2064	ARG	NE-CZ-NH2	-8.51	116.05	120.30
3	C	3102	ARG	NE-CZ-NH2	-8.01	116.30	120.30
3	C	3152	ARG	NE-CZ-NH2	7.79	124.19	120.30
2	E	5011	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	D	4491	ARG	NE-CZ-NH1	-7.41	116.60	120.30
3	C	3175	ARG	NE-CZ-NH2	7.39	124.00	120.30
2	B	2384	ARG	NE-CZ-NH2	7.39	123.99	120.30
2	E	5028	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	D	4421	ARG	NH1-CZ-NH2	-7.13	111.55	119.40
3	C	3068	ARG	CD-NE-CZ	7.09	133.52	123.60
2	B	2117	ARG	NE-CZ-NH2	-7.02	116.79	120.30
3	F	6121	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	1284	ARG	NE-CZ-NH2	6.96	123.78	120.30
3	F	6152	ARG	NE-CZ-NH2	6.96	123.78	120.30
3	F	6121	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	4063	ARG	NE-CZ-NH2	-6.81	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3175	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	1563	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	D	4116	ARG	CD-NE-CZ	6.78	133.10	123.60
3	C	3235	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	E	5117	ARG	NE-CZ-NH1	-6.70	116.95	120.30
3	C	3235	ARG	NE-CZ-NH2	-6.70	116.95	120.30
3	F	6152	ARG	NE-CZ-NH1	-6.65	116.97	120.30
3	C	3068	ARG	NE-CZ-NH1	6.64	123.62	120.30
3	F	6068	ARG	CD-NE-CZ	6.62	132.86	123.60
2	B	2069	ARG	NE-CZ-NH2	-6.61	116.99	120.30
3	C	3152	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	D	4284	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	D	4491	ARG	NE-CZ-NH2	6.32	123.46	120.30
3	C	3018	ARG	NE-CZ-NH1	-6.20	117.20	120.30
3	F	6212	ARG	CD-NE-CZ	6.17	132.23	123.60
1	A	1081	ARG	CD-NE-CZ	6.13	132.19	123.60
3	C	3019	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	D	4551[A]	ARG	CD-NE-CZ	5.69	131.56	123.60
1	D	4551[B]	ARG	CD-NE-CZ	5.69	131.56	123.60
3	C	3240	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	E	5117	ARG	NE-CZ-NH2	5.57	123.09	120.30
3	C	3121	ARG	CD-NE-CZ	5.57	131.40	123.60
1	A	1063	ARG	NE-CZ-NH2	-5.55	117.53	120.30
3	C	3127	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	1491	ARG	NE-CZ-NH1	-5.46	117.57	120.30
3	C	3111	ARG	NE-CZ-NH1	-5.43	117.59	120.30
2	B	2069	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	F	6212	ARG	CG-CD-NE	5.40	123.14	111.80
3	F	6102	ARG	NE-CZ-NH2	-5.38	117.61	120.30
3	F	6084	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	4519	ARG	CD-NE-CZ	5.30	131.01	123.60
2	B	2011	ARG	NE-CZ-NH1	-5.29	117.66	120.30
3	F	6068	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	1547	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	4460	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	4063	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	4460	ARG	CG-CD-NE	5.13	122.57	111.80
1	D	4081	ARG	CD-NE-CZ	5.07	130.69	123.60
2	E	5272	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	4287	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2331	TYR	Sidechain
2	B	2347	TYR	Sidechain
3	C	3093	TYR	Sidechain
2	E	5148	TYR	Sidechain
2	E	5331	TYR	Sidechain
2	E	5347	TYR	Sidechain
3	F	6093	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4346	0	4191	39	0
1	D	4348	0	4205	50	0
2	B	3176	0	3161	17	0
2	E	3178	0	3170	22	0
3	C	1947	0	1888	9	0
3	F	1950	0	1894	13	0
4	A	62	0	43	6	0
4	D	62	0	43	5	0
5	A	21	0	19	2	0
5	D	21	0	19	1	0
6	A	7	0	5	1	0
6	D	7	0	5	0	0
7	A	12	0	16	0	0
7	D	6	0	8	0	0
8	A	489	0	0	5	0
8	B	342	0	0	1	0
8	C	241	0	0	1	0
8	D	522	0	0	4	0
8	E	339	0	0	4	0
8	F	264	0	0	2	0
All	All	21340	0	18667	131	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 (131) 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:D:4551[B]:ARG:CZ	1:D:4551[B]:ARG:NH2	1.69	1.56
1:D:4551[B]:ARG:CG	1:D:4551[B]:ARG:CD	1.76	1.55
1:D:4551[B]:ARG:CG	1:D:4551[B]:ARG:NE	1.87	1.38
1:D:4551[B]:ARG:CB	1:D:4551[B]:ARG:CD	2.38	1.01
1:D:4551[B]:ARG:HG2	1:D:4551[B]:ARG:HE	1.24	1.01
1:D:4551[B]:ARG:NE	1:D:4551[B]:ARG:HG2	1.76	0.92
1:D:4551[B]:ARG:CG	1:D:4551[B]:ARG:HE	1.73	0.90
1:D:4551[B]:ARG:NE	1:D:4551[B]:ARG:NH2	2.31	0.74
1:D:4551[A]:ARG:NH2	1:D:4557:PHE:HA	2.02	0.72
1:D:4551[B]:ARG:HB2	1:D:4551[B]:ARG:CD	2.18	0.72
2:B:2048:ALA:HB2	2:B:2107:LYS:HD2	1.74	0.70
4:A:2570:F43:H9A1	1:D:4341:VAL:HB	1.74	0.68
1:D:4551[B]:ARG:HH11	1:D:4551[B]:ARG:HH21	0.66	0.66
1:A:1341:VAL:HB	4:D:5570:F43:H9A1	1.78	0.66
1:D:4369:ASP:HB3	8:D:2386:HOH:O	1.96	0.65
2:B:2403[B]:MET:SD	1:D:4132:LYS:HD3	2.38	0.64
1:D:4551[B]:ARG:NH2	1:D:4551[B]:ARG:HH12	1.15	0.63
2:E:5037:MET:HG2	2:E:5115:LYS:HE2	1.82	0.62
2:E:5099:ASN:HD21	2:E:5101:ILE:HD11	1.66	0.61
1:A:1053:ILE:HG12	1:A:1070:PRO:HG2	1.84	0.60
1:D:4020:GLU:HB3	8:D:2030:HOH:O	2.03	0.59
1:D:4551[B]:ARG:NH1	1:D:4551[B]:ARG:NH2	0.58	0.58
1:A:1465:GL3:HA2	2:B:2355:VAL:HG12	1.86	0.57
1:D:4125:MET:HE1	1:D:4272:ALA:HB3	1.86	0.57
3:C:3085:TYR:CE2	1:D:4256:CYS:HB2	2.41	0.55
2:B:2241:GLN:HE22	2:B:2386:PHE:HA	1.71	0.55
1:A:1145:HIS:HD2	8:A:2146:HOH:O	1.90	0.54
1:D:4551[B]:ARG:HH22	1:D:4551[B]:ARG:HH12	0.75	0.53
1:D:4551[B]:ARG:NH1	1:D:4551[B]:ARG:HH21	1.36	0.53
3:F:6037:LEU:O	3:F:6040[B]:VAL:HG12	2.09	0.53
1:D:4551[B]:ARG:HH11	1:D:4551[B]:ARG:NH2	0.58	0.52
2:B:2297:VAL:HB	2:B:2298:PRO:HD3	1.90	0.52
1:A:1256:CYS:HB2	3:F:6085:TYR:CE2	2.45	0.52
3:F:6096:PRO:HA	3:F:6213:THR:HA	1.91	0.52
2:E:5297:VAL:HB	2:E:5298:PRO:HD3	1.92	0.51
1:A:1239:ARG:O	1:A:1243:MET:HG2	2.10	0.51
1:A:1057:LYS:HE2	8:A:2073:HOH:O	2.11	0.51
2:E:5254:LYS:HD3	8:E:2249:HOH:O	2.10	0.51
1:A:1257:ALA:HB1	4:A:2570:F43:H9B1	1.92	0.50
1:D:4551[B]:ARG:NH1	1:D:4551[B]:ARG:HH22	1.01	0.50
1:D:4465:GL3:HA2	2:E:5355:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:GLN:HA	1:A:1348:THR:OG1	2.11	0.50
1:A:1197:ASP:HB3	1:A:1200:LYS:HB3	1.94	0.50
1:D:4297:PHE:HB3	1:D:4509:ALA:HA	1.94	0.49
1:D:4257:ALA:HB1	4:D:5570:F43:H9B1	1.93	0.49
1:D:4053:ILE:HG12	1:D:4070:PRO:HG2	1.95	0.49
2:B:2126:SER:HB3	2:E:5222:GLU:HG3	1.94	0.49
2:B:2188:SER:HB2	2:E:5122:ALA:HB3	1.96	0.48
1:A:1516:HIS:HB3	1:A:1521:ASP:HB2	1.96	0.47
2:E:5199:ALA:HB2	2:E:5406:ILE:HG23	1.95	0.47
1:D:4239:ARG:O	1:D:4243:MET:HG2	2.14	0.47
2:B:2180:GLN:HA	2:E:5180:GLN:HA	1.96	0.47
3:C:3096:PRO:HA	3:C:3213:THR:HA	1.97	0.47
3:F:6147:ALA:HB2	3:F:6203:PRO:HB3	1.96	0.47
1:D:4197:ASP:HB3	1:D:4200:LYS:HB3	1.97	0.47
1:A:1125:MET:HE1	8:E:2147:HOH:O	2.15	0.47
1:D:4551[B]:ARG:CB	1:D:4551[B]:ARG:HD3	2.41	0.46
1:D:4257:ALA:HB1	4:D:5570:F43:HAB1	1.98	0.46
1:A:1132:LYS:HD3	2:E:5403:MET:SD	2.55	0.46
2:E:5009:ASP:HB3	2:E:5015:LEU:HD11	1.97	0.46
3:F:6118:LEU:HD22	3:F:6121:ARG:HD3	1.98	0.46
1:A:1297:PHE:HB3	1:A:1509:ALA:HA	1.97	0.46
1:A:1467:ASP:HB2	1:A:1470:ASP:HB2	1.98	0.46
2:B:2199:ALA:HB2	2:B:2406:ILE:HG23	1.97	0.46
1:D:4125:MET:HE1	1:D:4272:ALA:CB	2.47	0.45
4:A:2570:F43:O8D	1:D:4417:GLY:HA3	2.16	0.45
2:E:5202:ASN:HB3	8:E:2218:HOH:O	2.16	0.45
1:A:1369:ASP:HB3	8:A:2300:HOH:O	2.17	0.45
1:A:1257:ALA:HB1	4:A:2570:F43:HAB1	1.99	0.45
3:F:6133:GLN:NE2	8:F:2158:HOH:O	2.49	0.45
1:A:1165:VAL:O	1:D:4341:VAL:HG13	2.17	0.45
1:D:4516:HIS:HB3	1:D:4521:ASP:HB2	1.99	0.45
2:B:2342:LEU:HD23	3:C:3239:GLN:HE22	1.83	0.44
2:E:5240:TYR:HB3	2:E:5306:VAL:CG2	2.48	0.44
2:E:5419:ALA:HB3	8:E:2333:HOH:O	2.17	0.44
1:A:1125:MET:HB2	8:A:2117:HOH:O	2.16	0.44
1:A:1268:ALA:HA	1:A:1272:ALA:HB3	2.00	0.44
2:B:2253:VAL:HG21	2:B:2313:LEU:HD12	1.99	0.44
1:D:4467:ASP:HB2	1:D:4470:ASP:HB2	1.99	0.44
1:D:4473:GLY:O	1:D:4477:VAL:HG23	2.17	0.44
3:C:3147:ALA:HB2	3:C:3203:PRO:HB3	1.99	0.44
3:C:3004:GLU:HG3	8:C:2002:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6097:ALA:HB2	3:F:6143:ILE:O	2.18	0.44
2:B:2122:ALA:HB3	2:E:5188:SER:HB2	1.99	0.43
2:B:2222:GLU:HG3	2:E:5126:SER:HB3	1.99	0.43
2:E:5312:THR:HA	2:E:5328:THR:HG21	2.00	0.43
2:B:2422:GLU:HG2	8:B:3035:HOH:O	2.19	0.43
1:A:1140:PRO:HB3	1:A:1189:GLU:HB3	2.00	0.43
3:C:3118:LEU:HD12	3:C:3118:LEU:N	2.34	0.43
1:A:1526:ASN:HA	1:A:1527:PRO:HD2	1.86	0.43
1:D:4345:GLN:HA	1:D:4348:THR:OG1	2.18	0.43
2:E:5037:MET:SD	2:E:5115:LYS:HG2	2.59	0.43
2:B:2346:ASP:HB3	2:B:2349:LYS:HB2	2.01	0.42
1:A:1312:ASP:HB3	1:A:1315:LYS:HB3	2.01	0.42
1:A:1568:PRO:HG2	1:D:4558:VAL:HG22	2.01	0.42
1:A:1231:THR:HG23	8:D:2117:HOH:O	2.20	0.42
1:A:1325:CYS:O	1:A:1329:ASP:HB2	2.19	0.42
5:A:2571:TP7:O3P	1:D:4271:MHS:NE2	2.52	0.42
1:A:1136:LYS:HE2	1:A:1253:TYR:O	2.20	0.42
3:C:3100:TYR:CD2	3:C:3117:THR:HG21	2.54	0.42
1:A:1341:VAL:HG13	1:D:4165:VAL:O	2.19	0.42
1:A:1293:GLY:HA2	1:A:1493:PRO:HB2	2.01	0.42
1:A:1472:SMC:SG	2:B:2349:LYS:HA	2.60	0.42
3:C:3127:ARG:HB2	3:C:3130:ASP:OD1	2.20	0.42
4:A:2570:F43:H5D2	1:D:4346:TYR:CZ	2.54	0.42
1:D:4233:ASP:O	1:D:4236:GLN:HB3	2.20	0.42
4:A:2570:F43:H5D2	1:D:4346:TYR:CE2	2.56	0.41
3:F:6055:PRO:HB2	3:F:6060:MET:HG3	2.02	0.41
3:F:6213:THR:OG1	3:F:6215:ILE:HG22	2.20	0.41
1:A:1326:MET:O	1:A:1330:GLN:HB2	2.20	0.41
1:A:1493:PRO:O	1:A:1499:ALA:HA	2.21	0.41
1:A:1525:VAL:O	2:E:5064:ARG:HA	2.20	0.41
1:D:4346:TYR:HE1	1:D:4419:SER:HB2	1.85	0.41
1:A:1463:PHE:HB2	6:A:2572:COM:O1S	2.21	0.41
3:F:6100:TYR:CD2	3:F:6117:THR:HG21	2.55	0.41
1:D:4472:SMC:SG	2:E:5349:LYS:HA	2.61	0.41
1:A:1463:PHE:CZ	5:A:2571:TP7:S7	3.14	0.41
2:E:5337:GLU:HG2	2:E:5342:LEU:O	2.20	0.41
3:C:3097:ALA:HB2	3:C:3143:ILE:O	2.20	0.41
1:D:4551[B]:ARG:HB2	1:D:4551[B]:ARG:HD3	1.99	0.41
1:A:1486:LEU:HD22	2:E:5162:PRO:HD2	2.03	0.41
2:B:2240:TYR:HB3	2:B:2306:VAL:CG2	2.50	0.41
1:A:1417:GLY:HA3	4:D:5570:F43:O8D	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5570:F43:CHC	4:D:5570:F43:HBB1	2.50	0.40
1:A:1057:LYS:HE3	8:A:2072:HOH:O	2.21	0.40
1:D:4002:ALA:HB1	8:D:2175:HOH:O	2.22	0.40
1:D:4334:GLY:HA2	1:D:4343:PHE:CD2	2.57	0.40
3:F:6136:LYS:HE2	8:F:2081:HOH:O	2.20	0.40
1:D:4035:THR:HA	3:F:6163:LEU:O	2.21	0.40
3:F:6036:ASP:O	3:F:6040[A]:VAL:HG23	2.22	0.40
1:A:1271:MHS:NE2	5:D:5571:TP7:O3P	2.55	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	566/569 (100%)	546 (96%)	19 (3%)	1 (0%)	52	28
1	D	565/569 (99%)	546 (97%)	18 (3%)	1 (0%)	52	28
2	B	434/433 (100%)	428 (99%)	6 (1%)	0	100	100
2	E	432/433 (100%)	426 (99%)	6 (1%)	0	100	100
3	C	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
3	F	245/247 (99%)	237 (97%)	8 (3%)	0	100	100
All	All	2486/2498 (100%)	2422 (97%)	62 (2%)	2 (0%)	56	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1525	VAL
1	D	4525	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/443 (101%)	436 (98%)	10 (2%)	60	31
1	D	445/443 (100%)	436 (98%)	9 (2%)	63	36
2	B	335/332 (101%)	333 (99%)	2 (1%)	90	82
2	E	333/332 (100%)	331 (99%)	2 (1%)	90	82
3	C	201/201 (100%)	197 (98%)	4 (2%)	63	36
3	F	202/201 (100%)	198 (98%)	4 (2%)	63	36
All	All	1962/1952 (100%)	1931 (98%)	31 (2%)	72	47

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

Mol	Chain	Res	Type
1	A	1008	LYS
1	A	1061	GLU
1	A	1102	TYR
1	A	1141	GLU
1	A	1204	GLU
1	A	1335	SER
1	A	1359	ASN
1	A	1369	ASP
1	A	1384	LYS
1	A	1464	PHE
2	B	2093[A]	ASP
2	B	2093[B]	ASP
3	C	3122	GLN
3	C	3176	ARG
3	C	3178	LEU
3	C	3196	ARG
1	D	4102	TYR
1	D	4131	GLU
1	D	4335	SER
1	D	4359	ASN
1	D	4369	ASP
1	D	4464	PHE

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Mol	Chain	Res	Type
1	D	4525	VAL
1	D	4551[A]	ARG
1	D	4551[B]	ARG
2	E	5062	LYS
2	E	5103	VAL
3	F	6176	ARG
3	F	6178	LEU
3	F	6195	ASP
3	F	6196	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1145	HIS
1	A	1358	ASN
2	B	2202	ASN
2	B	2241	GLN
2	B	2402	GLN
3	C	3070	ASN
3	C	3122	GLN
3	C	3239	GLN
1	D	4019	GLN
2	E	5402	GLN
3	F	6070	ASN
3	F	6133	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	MHS	A	1271	1	8,11,12	1.75	1 (12%)	7,14,16	1.42	1 (14%)
1	AGM	A	1285	1	7,11,12	0.52	0	5,13,15	0.86	0
1	GL3	A	1465	1	3,3,4	2.89	1 (33%)	2,2,4	0.28	0
1	SMC	A	1472	1	5,6,7	0.60	0	2,6,8	1.32	0
3	OCS	C	3065	3	7,8,9	1.38	1 (14%)	7,11,13	1.92	2 (28%)
1	MHS	D	4271	1	8,11,12	1.75	1 (12%)	7,14,16	1.53	2 (28%)
1	AGM	D	4285	1	7,11,12	0.47	0	5,13,15	0.88	0
1	GL3	D	4465	1	3,3,4	2.86	1 (33%)	2,2,4	0.13	0
1	SMC	D	4472	1	5,6,7	0.59	0	2,6,8	1.38	0
3	OCS	F	6065	3	7,8,9	1.32	0	7,11,13	1.81	2 (28%)

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
1	MHS	A	1271	1	-	0/4/6/8	0/1/1/1
1	AGM	A	1285	1	-	0/7/11/13	0/0/0/0
1	GL3	A	1465	1	-	0/1/1/2	0/0/0/0
1	SMC	A	1472	1	-	0/3/5/7	0/0/0/0
3	OCS	C	3065	3	-	0/4/7/9	0/0/0/0
1	MHS	D	4271	1	-	0/4/6/8	0/1/1/1
1	AGM	D	4285	1	-	0/7/11/13	0/0/0/0
1	GL3	D	4465	1	-	0/1/1/2	0/0/0/0
1	SMC	D	4472	1	-	0/3/5/7	0/0/0/0
3	OCS	F	6065	3	-	0/4/7/9	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1465	GL3	C-S	-5.01	1.63	1.80
1	D	4465	GL3	C-S	-4.95	1.63	1.80
3	C	3065	OCS	OD1-SG	2.09	1.51	1.45
1	A	1271	MHS	CM-ND1	4.68	1.57	1.47
1	D	4271	MHS	CM-ND1	4.76	1.58	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4271	MHS	NE2-CE1-ND1	-2.32	109.14	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1271	MHS	NE2-CE1-ND1	-2.32	109.14	112.28
1	D	4271	MHS	O-C-CA	-2.21	119.74	125.49
3	C	3065	OCS	OD1-SG-CB	2.52	109.07	106.94
3	F	6065	OCS	OD1-SG-CB	2.85	109.34	106.94
3	F	6065	OCS	OD3-SG-CB	2.88	109.37	106.94
3	C	3065	OCS	OD3-SG-CB	3.59	109.97	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1271	MHS	1	0
1	A	1465	GL3	1	0
1	A	1472	SMC	1	0
1	D	4271	MHS	1	0
1	D	4465	GL3	1	0
1	D	4472	SMC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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
4	F43	A	2570	1,6	42,71,71	4.17	18 (42%)	35,118,118	2.15	7 (20%)
5	TP7	A	2571	-	16,20,20	2.01	2 (12%)	16,26,26	1.35	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	COM	A	2572	4	5,6,6	1.58	1 (20%)	5,8,8	1.63	1 (20%)
7	GOL	A	2573	-	5,5,5	1.01	0	5,5,5	0.53	0
7	GOL	A	2574	-	5,5,5	0.86	0	5,5,5	0.54	0
4	F43	D	5570	1,6	42,71,71	4.16	18 (42%)	35,118,118	2.17	7 (20%)
5	TP7	D	5571	-	16,20,20	2.01	2 (12%)	16,26,26	1.38	2 (12%)
6	COM	D	5572	4	5,6,6	1.54	1 (20%)	5,8,8	1.74	1 (20%)
7	GOL	D	5573	-	5,5,5	1.03	0	5,5,5	0.59	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
4	F43	A	2570	1,6	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	A	2571	-	1/1/5/6	0/20/24/24	0/0/0/0
6	COM	A	2572	4	-	0/4/4/4	0/0/0/0
7	GOL	A	2573	-	-	0/4/4/4	0/0/0/0
7	GOL	A	2574	-	-	0/4/4/4	0/0/0/0
4	F43	D	5570	1,6	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	D	5571	-	1/1/5/6	0/20/24/24	0/0/0/0
6	COM	D	5572	4	-	0/4/4/4	0/0/0/0
7	GOL	D	5573	-	-	0/4/4/4	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5570	F43	C4B-NB	-19.41	1.19	1.49
4	A	2570	F43	C4B-NB	-19.21	1.20	1.49
5	A	2571	TP7	C2-C1	-6.01	1.39	1.51
5	D	5571	TP7	C2-C1	-5.96	1.39	1.51
4	D	5570	F43	C1D-ND	-3.51	1.29	1.36
4	A	2570	F43	C1D-ND	-3.50	1.29	1.36
4	D	5570	F43	C4A-NA	-2.73	1.44	1.49
4	A	2570	F43	C4A-NA	-2.68	1.44	1.49
4	D	5570	F43	C6B-N5B	-2.57	1.30	1.34
4	A	2570	F43	C6B-N5B	-2.48	1.30	1.34
4	A	2570	F43	C9A-C2A	-2.38	1.50	1.54
4	D	5570	F43	C8B-C2B	-2.38	1.51	1.54
4	A	2570	F43	C8B-C2B	-2.36	1.51	1.54
4	D	5570	F43	C9A-C2A	-2.30	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5570	F43	C5D-C2D	-2.26	1.48	1.51
4	A	2570	F43	C5D-C2D	-2.11	1.48	1.51
6	D	5572	COM	O3S-S2	2.36	1.52	1.46
6	A	2572	COM	O3S-S2	2.41	1.52	1.46
4	D	5570	F43	C1B-NB	2.69	1.53	1.49
4	A	2570	F43	C1B-NB	3.06	1.54	1.49
4	D	5570	F43	C1D-C2D	3.13	1.49	1.40
5	A	2571	TP7	C1-N	3.17	1.40	1.34
4	A	2570	F43	C1D-C2D	3.22	1.49	1.40
4	D	5570	F43	CHD-C7D	3.39	1.54	1.46
5	D	5571	TP7	C1-N	3.46	1.41	1.34
4	A	2570	F43	CHD-C7D	3.48	1.54	1.46
4	D	5570	F43	NI-NC	3.56	2.06	1.90
4	A	2570	F43	NI-NC	3.65	2.06	1.90
4	D	5570	F43	C1B-N5B	3.99	1.54	1.45
4	A	2570	F43	C1B-N5B	4.04	1.54	1.45
4	D	5570	F43	CAB-C3B	4.22	1.62	1.53
4	A	2570	F43	C2B-C3B	4.38	1.62	1.54
4	A	2570	F43	CAB-C3B	4.40	1.63	1.53
4	D	5570	F43	CAA-C3A	4.41	1.63	1.53
4	D	5570	F43	C2B-C3B	4.43	1.62	1.54
4	A	2570	F43	CAA-C3A	4.48	1.63	1.53
4	D	5570	F43	C4D-C3D	7.10	1.47	1.37
4	A	2570	F43	C3D-C2D	7.17	1.55	1.39
4	D	5570	F43	C3D-C2D	7.30	1.55	1.39
4	A	2570	F43	C4D-C3D	7.38	1.47	1.37
4	D	5570	F43	C2A-C1A	8.28	1.62	1.51
4	A	2570	F43	C2A-C1A	8.55	1.63	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5570	F43	C9D-C3D-C4D	-7.50	114.37	127.01
4	A	2570	F43	C9D-C3D-C4D	-7.45	114.46	127.01
4	D	5570	F43	O8D-C7D-C6D	-4.10	113.32	120.76
4	A	2570	F43	O8D-C7D-C6D	-4.06	113.39	120.76
5	D	5571	TP7	O1-C1-N	-3.34	117.35	123.01
5	A	2571	TP7	O1-C1-N	-3.29	117.43	123.01
4	A	2570	F43	C4A-NA-C1A	2.00	110.22	108.21
4	D	5570	F43	C4A-NA-C1A	2.01	110.23	108.21
5	A	2571	TP7	C4-C3-C2	2.26	121.59	113.29
5	D	5571	TP7	C4-C3-C2	2.35	121.89	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2570	F43	C9B-C2B-C3B	2.43	116.60	111.81
4	D	5570	F43	C9B-C2B-C3B	2.59	116.92	111.81
4	D	5570	F43	C3A-C4A-NA	2.66	106.57	102.27
4	A	2570	F43	C3A-C4A-NA	2.73	106.68	102.27
6	A	2572	COM	O2S-S2-C2	2.97	109.44	106.91
6	D	5572	COM	O2S-S2-C2	3.30	109.72	106.91
4	D	5570	F43	C8B-C2B-C1B	3.32	108.25	102.05
4	A	2570	F43	C8B-C2B-C1B	3.32	108.26	102.05
4	A	2570	F43	C3B-C4B-NB	5.90	124.45	106.03
4	D	5570	F43	C3B-C4B-NB	5.91	124.48	106.03

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	5571	TP7	C1
4	D	5570	F43	C4B
5	A	2571	TP7	C1
4	A	2570	F43	C4B

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2570	F43	6	0
5	A	2571	TP7	2	0
6	A	2572	COM	1	0
4	D	5570	F43	5	0
5	D	5571	TP7	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	564/569 (99%)	-0.49	7 (1%) 81 81	7, 12, 22, 36	0
1	D	564/569 (99%)	-0.53	4 (0%) 89 89	7, 11, 20, 36	0
2	B	432/433 (99%)	-0.45	4 (0%) 85 85	8, 12, 24, 42	0
2	E	433/433 (100%)	-0.48	3 (0%) 89 89	8, 12, 22, 37	0
3	C	246/247 (99%)	-0.33	4 (1%) 74 74	9, 15, 24, 35	0
3	F	246/247 (99%)	-0.38	6 (2%) 62 60	10, 14, 24, 39	0
All	All	2485/2498 (99%)	-0.47	28 (1%) 82 83	7, 12, 23, 42	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4569	ALA	9.4
1	A	1569	ALA	8.3
3	C	3002	ALA	6.1
3	C	3064	ALA	4.8
2	B	2433	VAL	4.4
3	F	6002	ALA	4.1
3	F	6064	ALA	3.9
2	E	5434	LEU	3.7
3	F	6196	ARG	3.2
2	E	5104	LYS	3.0
3	C	3196	ARG	2.9
2	E	5105	GLY	2.7
1	D	4369	ASP	2.7
1	A	1369	ASP	2.6
3	F	6207	GLU	2.6
1	A	1003	ALA	2.5
2	B	2002	SER	2.5
2	B	2104	LYS	2.5
3	F	6195	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	6180	ASN	2.4
3	C	3180	ASN	2.4
1	A	1027	THR	2.3
1	D	4002	ALA	2.2
1	A	1372	ASN	2.2
1	A	1388	GLU	2.1
1	D	4372	ASN	2.1
1	A	1384	LYS	2.0
2	B	2415	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
3	OCS	C	3065	9/10	0.95	0.10	-	19,24,26,26	0
1	GL3	A	1465	4/5	0.99	0.05	-	9,9,9,9	0
1	SMC	D	4472	7/8	0.99	0.05	-	9,10,10,10	0
1	GL3	D	4465	4/5	0.99	0.05	-	8,8,8,8	0
1	MHS	D	4271	11/12	0.97	0.06	-	10,11,12,13	0
1	MHS	A	1271	11/12	0.97	0.05	-	9,10,12,12	0
1	AGM	A	1285	12/13	0.98	0.07	-	6,7,8,8	0
1	AGM	D	4285	12/13	0.98	0.08	-	6,7,8,8	0
3	OCS	F	6065	9/10	0.97	0.07	-	18,22,25,25	0
1	SMC	A	1472	7/8	0.99	0.05	-	9,9,10,11	0

## 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( $\text{\AA}^2$ )	Q<0.9
7	GOL	D	5573	6/6	0.71	0.25	11.39	30,32,33,35	0
7	GOL	A	2573	6/6	0.77	0.20	9.82	33,34,35,37	0
7	GOL	A	2574	6/6	0.68	0.25	7.77	36,38,39,40	0
6	COM	D	5572	7/7	0.95	0.11	6.67	16,17,17,18	0
6	COM	A	2572	7/7	0.95	0.10	5.77	15,16,17,18	0
4	F43	D	5570	62/62	0.98	0.07	1.39	8,10,12,13	0
4	F43	A	2570	62/62	0.98	0.07	1.36	8,10,11,14	0
5	TP7	A	2571	21/21	0.98	0.07	0.14	8,8,10,12	0
5	TP7	D	5571	21/21	0.98	0.07	0.04	7,9,10,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.