



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:34 PM BST

PDB ID : 6DEW  
Title : Structure of human COQ9 protein with bound isoprene.  
Authors : Bingman, C.A.; Lohman, D.C.; Smith, R.W.; Pagliarini, D.J.  
Deposited on : 2018-05-13  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

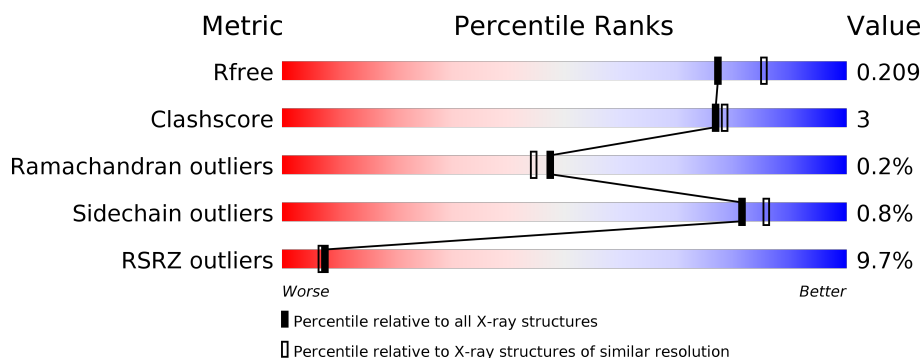
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	212	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	212	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	212	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>11%</div> </div> </div>
1	D	212	<div> <div>17%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
1	E	212	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>10%</div> </div> </div>
1	F	212	<div> <div>14%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>13%</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
3	64Z	B	302	-	-	-	X
5	FOF	A	304	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18799 atoms, of which 9056 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 Ubiquinone biosynthesis protein COQ9, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	H	N	O	S	0	1	0
			3095	988	1522	272	301	12			
1	B	191	Total	C	H	N	O	S	0	1	0
			3033	967	1493	268	294	11			
1	C	188	Total	C	H	N	O	S	0	2	0
			3002	957	1478	264	293	10			
1	D	189	Total	C	H	N	O	S	0	1	0
			3010	959	1485	264	290	12			
1	E	191	Total	C	H	N	O	S	0	1	0
			3032	966	1496	268	290	12			
1	F	184	Total	C	H	N	O	S	0	1	0
			2934	935	1450	258	279	12			

There are 18 discrepancies between the modelled and reference sequences:

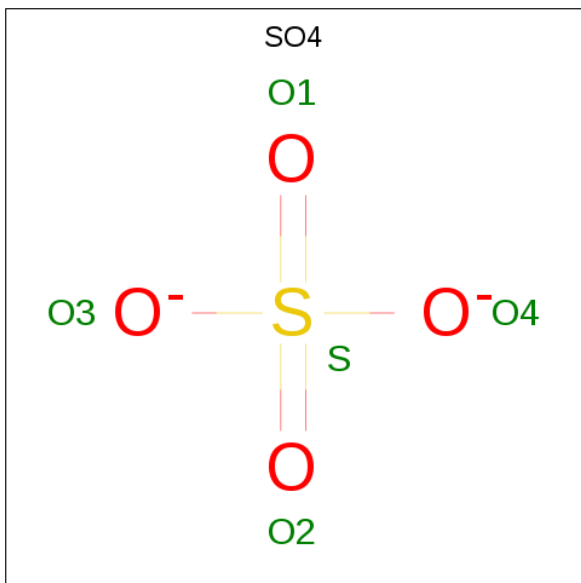
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	SER	-	expression tag	UNP O75208
A	77	HIS	-	expression tag	UNP O75208
A	78	MET	-	expression tag	UNP O75208
B	76	SER	-	expression tag	UNP O75208
B	77	HIS	-	expression tag	UNP O75208
B	78	MET	-	expression tag	UNP O75208
C	76	SER	-	expression tag	UNP O75208
C	77	HIS	-	expression tag	UNP O75208
C	78	MET	-	expression tag	UNP O75208
D	76	SER	-	expression tag	UNP O75208
D	77	HIS	-	expression tag	UNP O75208
D	78	MET	-	expression tag	UNP O75208
E	76	SER	-	expression tag	UNP O75208
E	77	HIS	-	expression tag	UNP O75208
E	78	MET	-	expression tag	UNP O75208
F	76	SER	-	expression tag	UNP O75208
F	77	HIS	-	expression tag	UNP O75208

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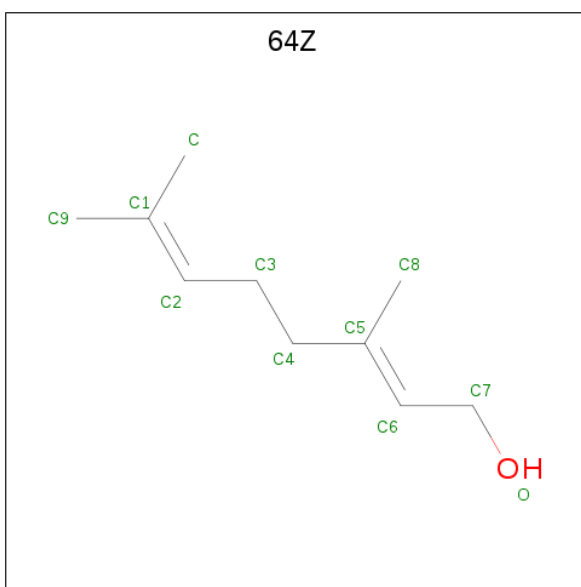
Chain	Residue	Modelled	Actual	Comment	Reference
F	78	MET	-	expression tag	UNP O75208

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



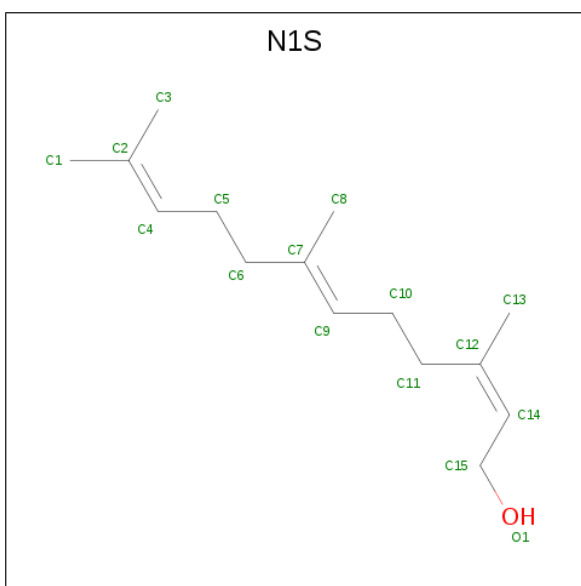
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is Geraniol (three-letter code: 64Z) (formula: C<sub>10</sub>H<sub>18</sub>O).



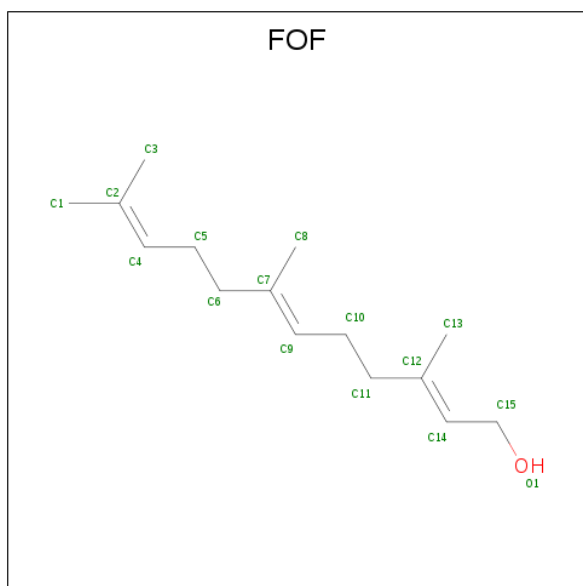
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			29	10	18	1		
3	B	1	Total	C	H	O	0	0
			29	10	18	1		
3	D	1	Total	C	H	O	0	0
			29	10	18	1		

- Molecule 4 is (2Z,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-ol (three-letter code: N1S) (formula: C<sub>15</sub>H<sub>26</sub>O).



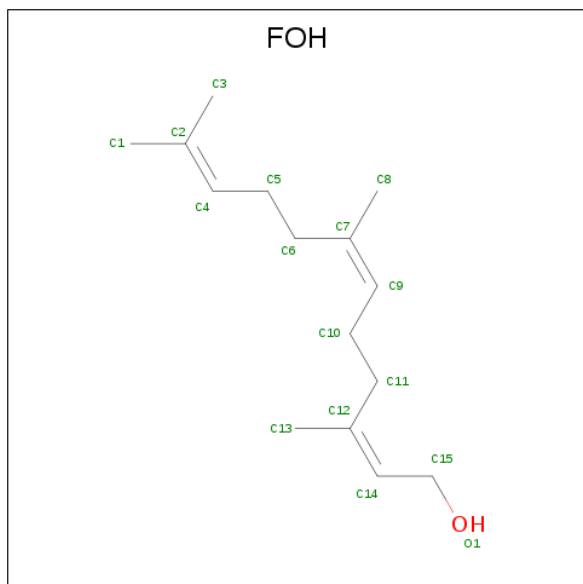
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			42	15	26	1		

- Molecule 5 is (2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-ol (three-letter code: FOF) (formula:  $C_{15}H_{26}O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			42	15	26	1		

- Molecule 6 is (2Z,6Z)-3,7,11-trimethyldodeca-2,6,10-trien-1-ol (three-letter code: FOH) (formula:  $C_{15}H_{26}O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			42	15	26	1		

- Molecule 7 is water.

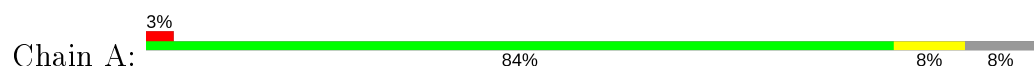
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	93	Total	O	0	0
			93	93		
7	B	101	Total	O	0	0
			101	101		
7	C	82	Total	O	0	0
			82	82		
7	D	54	Total	O	0	0
			54	54		
7	E	79	Total	O	0	0
			79	79		
7	F	46	Total	O	0	0
			46	46		



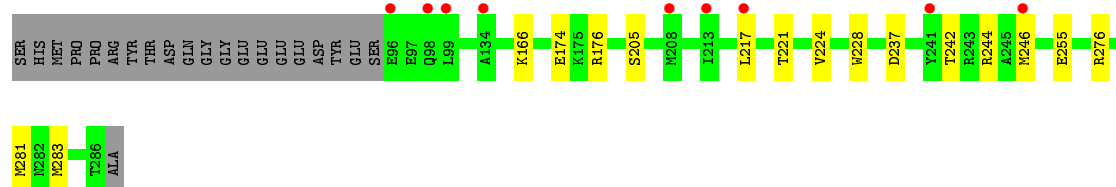
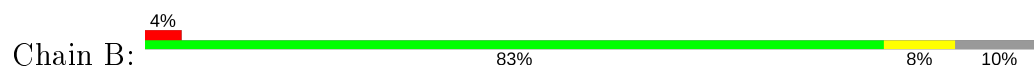
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

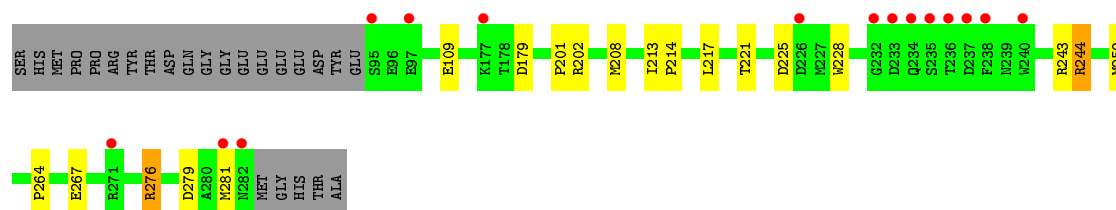
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



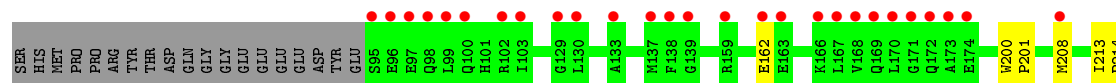
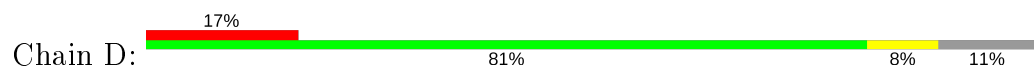
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial

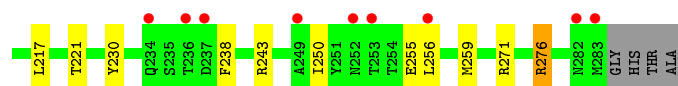


- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial

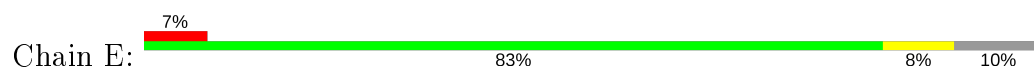


- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial

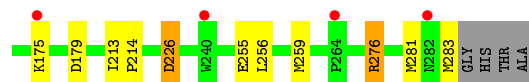
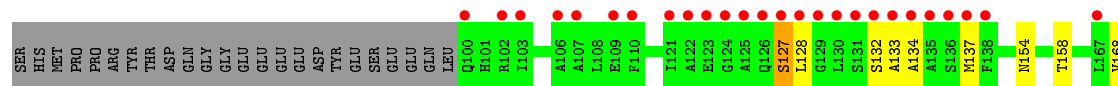
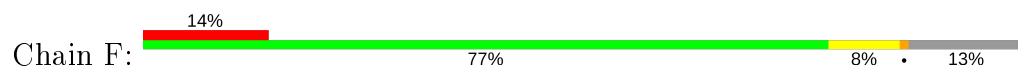




- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.45Å 222.78Å 130.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.00 48.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.00-2.00) 94.8 (48.00-2.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.169 , 0.209 0.169 , 0.209	Depositor DCC
$R_{free}$ test set	2045 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.333 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: N1S, FOF, 64Z, FOH, SO4

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	1.00	6/1607 (0.4%)	0.88	4/2177 (0.2%)
1	B	0.95	5/1573 (0.3%)	0.90	6/2133 (0.3%)
1	C	0.84	1/1556 (0.1%)	0.80	1/2111 (0.0%)
1	D	0.77	1/1557 (0.1%)	0.72	0/2110
1	E	0.94	6/1569 (0.4%)	0.84	2/2127 (0.1%)
1	F	0.75	1/1516 (0.1%)	0.74	0/2055
All	All	0.88	20/9378 (0.2%)	0.81	13/12713 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	VAL	CB-CG1	8.02	1.69	1.52
1	B	255	GLU	CG-CD	7.68	1.63	1.51
1	A	259	MET	CB-CG	6.53	1.72	1.51
1	A	224	VAL	CB-CG2	-6.51	1.39	1.52
1	B	224	VAL	CB-CG1	-6.33	1.39	1.52
1	A	251	TYR	CD2-CE2	6.19	1.48	1.39
1	C	208	MET	CB-CG	6.17	1.71	1.51
1	B	174	GLU	CG-CD	6.03	1.60	1.51
1	E	255	GLU	CG-CD	5.68	1.60	1.51
1	E	243	ARG	CB-CG	-5.68	1.37	1.52
1	E	224	VAL	CB-CG2	-5.54	1.41	1.52
1	A	223	MET	CG-SD	-5.34	1.67	1.81
1	E	251	TYR	CE2-CZ	-5.23	1.31	1.38
1	B	228	TRP	CE3-CZ3	5.15	1.47	1.38
1	B	205	SER	CB-OG	-5.13	1.35	1.42
1	D	255	GLU	CG-CD	5.13	1.59	1.51
1	A	255	GLU	CG-CD	5.11	1.59	1.51
1	F	255	GLU	CG-CD	5.07	1.59	1.51
1	E	174	GLU	CB-CG	5.05	1.61	1.52
1	E	164	GLU	CG-CD	5.04	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	B	176	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	A	225	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	102	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	B	237	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	102	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	237	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	202	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	E	243	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	A	225	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	281	MET	CG-SD-CE	5.21	108.54	100.20
1	B	244	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	E	261	ASP	CB-CG-OD2	-5.15	113.67	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1573	1522	1521	6	0
1	B	1540	1493	1491	12	0
1	C	1524	1478	1476	10	0
1	D	1525	1485	1484	10	0
1	E	1536	1496	1495	14	0
1	F	1484	1450	1448	13	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	11	18	0	0	0
3	B	11	18	0	0	0
3	D	11	18	0	0	0
4	A	16	26	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	16	26	0	0	0
6	D	16	26	26	1	0
7	A	93	0	0	0	0
7	B	101	0	0	0	0
7	C	82	0	0	1	0
7	D	54	0	0	0	0
7	E	79	0	0	0	0
7	F	46	0	0	0	0
All	All	9743	9056	8941	55	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 (55) 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:B:246:MET:HG2	1:E:246[B]:MET:HG2	1.67	0.76
1:B:246:MET:HG2	1:E:246[B]:MET:CG	2.17	0.74
1:B:246:MET:CG	1:E:246[B]:MET:HG2	2.20	0.72
1:B:217:LEU:O	1:B:221:THR:HG23	1.93	0.69
1:F:134:ALA:HB1	1:F:137:MET:SD	2.34	0.67
1:B:246:MET:HG2	1:E:246[B]:MET:HE2	1.84	0.58
1:D:250:ILE:HD13	1:D:276:ARG:HB3	1.86	0.58
1:B:242:THR:O	1:B:246:MET:HG3	2.04	0.57
1:C:225:ASP:OD2	1:C:244:ARG:NH2	2.40	0.54
1:F:158:THR:HG22	1:F:226:ASP:OD2	2.07	0.54
1:D:256:LEU:HD23	1:D:259:MET:CE	2.39	0.53
1:B:246:MET:SD	1:E:246[B]:MET:CE	2.98	0.52
1:D:238:PHE:HB2	1:D:243:ARG:HB3	1.91	0.52
1:A:183:ARG:HG3	1:A:277:VAL:HG11	1.90	0.51
1:A:211:HIS:HB3	1:F:283:MET:HB3	1.91	0.51
1:C:201:PRO:HG3	1:C:259:MET:HE2	1.92	0.51
1:B:246:MET:SD	1:E:246[B]:MET:SD	3.09	0.50
1:F:168:VAL:HG11	1:F:175:LYS:HG2	1.92	0.50
1:C:276:ARG:NH1	1:C:279:ASP:OD2	2.45	0.49
1:E:242:THR:O	1:E:246[B]:MET:HG3	2.12	0.49
1:A:228:TRP:O	1:A:233:ASP:HB2	2.13	0.49
1:E:103:ILE:HD13	1:E:128:LEU:HD12	1.96	0.47
1:D:217:LEU:O	1:D:221:THR:HG23	2.15	0.47
1:F:154:ASN:O	1:F:158:THR:HG23	2.14	0.47
1:B:246:MET:CG	1:E:246[B]:MET:HE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:N	1:D:214:PRO:CD	2.79	0.46
1:F:168:VAL:HG11	1:F:175:LYS:CG	2.46	0.46
1:B:283:MET:CE	1:E:246[B]:MET:HE3	2.46	0.45
1:C:213:ILE:N	1:C:214:PRO:CD	2.79	0.45
1:F:179:ASP:HB3	1:F:281:MET:SD	2.57	0.45
1:C:228:TRP:CZ2	1:C:243:ARG:HB2	2.51	0.45
1:F:127:SER:C	1:F:128:LEU:HD23	2.37	0.44
1:A:209:LEU:O	1:A:213:ILE:HG13	2.18	0.44
1:F:276:ARG:NE	1:F:276:ARG:HA	2.32	0.44
1:F:256:LEU:HD23	1:F:259:MET:CE	2.48	0.44
1:C:225:ASP:OD1	1:C:244:ARG:NE	2.51	0.44
1:F:213:ILE:CG2	1:F:214:PRO:HD3	2.48	0.44
1:D:208[B]:MET:HE1	6:D:303:FOH:C4	2.48	0.43
1:F:213:ILE:HG23	1:F:214:PRO:HD3	2.00	0.43
1:F:132:SER:O	1:F:134:ALA:N	2.52	0.43
1:C:217:LEU:O	1:C:221[A]:THR:HG23	2.18	0.43
1:E:246[A]:MET:CE	1:E:281:MET:CE	2.97	0.42
1:C:109:GLU:HG3	7:C:346:HOH:O	2.19	0.42
1:C:264:PRO:O	1:C:267:GLU:HG3	2.20	0.42
1:A:246[A]:MET:CE	1:A:281:MET:HE2	2.50	0.42
1:E:200:TRP:N	1:E:201:PRO:CD	2.83	0.41
1:A:246[A]:MET:CE	1:A:281:MET:CE	2.99	0.41
1:E:122:ALA:HB1	1:E:132:SER:HB2	2.03	0.41
1:C:179:ASP:HB3	1:C:281:MET:SD	2.61	0.41
1:D:276:ARG:HA	1:D:276:ARG:HD3	1.81	0.41
1:B:283:MET:HE2	1:E:246[B]:MET:SD	2.61	0.41
1:D:162:GLU:HG2	1:D:230:TYR:OH	2.21	0.41
1:D:213:ILE:CG2	1:D:214:PRO:HD3	2.51	0.40
1:B:276:ARG:HA	1:B:276:ARG:NE	2.37	0.40
1:D:200:TRP:N	1:D:201:PRO:CD	2.84	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	194/212 (92%)	190 (98%)	3 (2%)	1 (0%)	29	23
1	B	190/212 (90%)	187 (98%)	3 (2%)	0	100	100
1	C	188/212 (89%)	187 (100%)	1 (0%)	0	100	100
1	D	188/212 (89%)	180 (96%)	8 (4%)	0	100	100
1	E	190/212 (90%)	188 (99%)	2 (1%)	0	100	100
1	F	183/212 (86%)	175 (96%)	7 (4%)	1 (0%)	29	23
All	All	1133/1272 (89%)	1107 (98%)	24 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ASP
1	F	133	ALA

### 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	169/183 (92%)	169 (100%)	0	100	100
1	B	166/183 (91%)	165 (99%)	1 (1%)	86	90
1	C	165/183 (90%)	163 (99%)	2 (1%)	71	76
1	D	165/183 (90%)	163 (99%)	2 (1%)	71	76
1	E	165/183 (90%)	165 (100%)	0	100	100
1	F	160/183 (87%)	157 (98%)	3 (2%)	57	61
All	All	990/1098 (90%)	982 (99%)	8 (1%)	81	86

All (8) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	166	LYS
1	C	244	ARG
1	C	276	ARG
1	D	271	ARG
1	D	276	ARG
1	F	127	SER
1	F	226	ASP
1	F	276	ARG

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	$\# Z  > 2$
6	FOH	D	303	-	15,15,15	0.86	1 (6%)	17,17,17	1.81	5 (29%)
5	FOF	A	304	-	15,15,15	0.78	0	17,17,17	1.77	4 (23%)
3	64Z	D	302	-	10,10,10	1.30	1 (10%)	11,11,11	2.48	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	64Z	B	302	-	10,10,10	0.96	0	11,11,11	2.16	4 (36%)
2	SO4	D	301	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	A	301	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	B	301	-	4,4,4	0.12	0	6,6,6	0.18	0
4	N1S	A	303	-	15,15,15	0.84	1 (6%)	17,17,17	1.52	4 (23%)
3	64Z	A	302	-	10,10,10	1.06	1 (10%)	11,11,11	1.97	4 (36%)
2	SO4	E	301	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	F	301	-	4,4,4	0.18	0	6,6,6	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FOH	D	303	-	-	4/15/15/15	-
5	FOF	A	304	-	-	3/15/15/15	-
3	64Z	D	302	-	-	4/9/9/9	-
4	N1S	A	303	-	-	5/15/15/15	-
3	64Z	A	302	-	-	1/9/9/9	-
3	64Z	B	302	-	-	3/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	64Z	C7-C6	2.72	1.53	1.50
3	A	302	64Z	C7-C6	2.54	1.53	1.50
6	D	303	FOH	C13-C12	2.05	1.55	1.50
4	A	303	N1S	C15-C14	2.01	1.52	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	64Z	C7-C6-C5	-4.99	119.43	127.21
3	D	302	64Z	C8-C5-C4	4.61	123.02	115.27
5	A	304	FOF	C10-C9-C7	-3.79	118.53	127.66
3	A	302	64Z	C7-C6-C5	-3.76	121.35	127.21
3	B	302	64Z	C7-C6-C5	-3.70	121.44	127.21
3	B	302	64Z	C8-C5-C4	3.70	121.49	115.27
6	D	303	FOH	C13-C12-C11	3.36	120.92	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	303	FOH	C8-C7-C6	3.16	120.59	115.27
6	D	303	FOH	C8-C7-C9	-3.10	115.73	123.68
5	A	304	FOF	C13-C12-C11	2.96	120.24	115.27
3	A	302	64Z	C8-C5-C4	2.93	120.20	115.27
4	A	303	N1S	C13-C12-C11	2.85	120.07	115.27
6	D	303	FOH	C15-C14-C12	-2.82	122.82	127.21
5	A	304	FOF	C11-C12-C14	-2.76	115.52	121.12
3	B	302	64Z	C-C1-C9	2.58	120.30	114.60
3	A	302	64Z	C-C1-C9	2.46	120.04	114.60
4	A	303	N1S	C13-C12-C14	-2.43	117.45	123.68
4	A	303	N1S	O1-C15-C14	-2.43	105.36	110.79
3	D	302	64Z	C4-C5-C6	-2.41	116.24	121.12
4	A	303	N1S	C10-C9-C7	-2.40	121.88	127.66
5	A	304	FOF	C8-C7-C6	2.39	119.30	115.27
6	D	303	FOH	C5-C4-C2	-2.38	119.62	127.75
3	D	302	64Z	C-C1-C9	2.29	119.67	114.60
3	D	302	64Z	C3-C2-C1	-2.11	120.52	127.75
3	B	302	64Z	C3-C2-C1	-2.06	120.70	127.75
3	A	302	64Z	C3-C2-C1	-2.03	120.82	127.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	303	FOH	C10-C11-C12-C13
5	A	304	FOF	C4-C5-C6-C7
5	A	304	FOF	C10-C11-C12-C13
5	A	304	FOF	C10-C11-C12-C14
3	D	302	64Z	C2-C3-C4-C5
3	D	302	64Z	C3-C4-C5-C6
3	D	302	64Z	C3-C4-C5-C8
4	A	303	N1S	C4-C5-C6-C7
3	A	302	64Z	C2-C3-C4-C5
6	D	303	FOH	C10-C11-C12-C14
6	D	303	FOH	C4-C5-C6-C7
4	A	303	N1S	C9-C10-C11-C12
6	D	303	FOH	C9-C10-C11-C12
3	B	302	64Z	C3-C4-C5-C8
3	B	302	64Z	C2-C3-C4-C5
4	A	303	N1S	C5-C6-C7-C8
3	D	302	64Z	C5-C6-C7-O
4	A	303	N1S	C12-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
4	A	303	N1S	C5-C6-C7-C9
3	B	302	64Z	C3-C4-C5-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	303	FOH	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	195/212 (91%)	0.27	6 (3%)	49	48	27, 40, 73, 104	0
1	B	191/212 (90%)	0.30	9 (4%)	31	30	27, 42, 73, 100	0
1	C	188/212 (88%)	0.38	15 (7%)	12	11	29, 45, 80, 98	0
1	D	189/212 (89%)	0.91	36 (19%)	1	1	28, 53, 106, 126	0
1	E	191/212 (90%)	0.40	14 (7%)	15	14	27, 42, 84, 110	0
1	F	184/212 (86%)	0.86	30 (16%)	1	1	31, 55, 109, 137	0
All	All	1138/1272 (89%)	0.52	110 (9%)	7	7	27, 45, 92, 137	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	PHE	12.2
1	F	134	ALA	9.8
1	D	283	MET	9.7
1	F	133	ALA	9.6
1	F	130	LEU	7.8
1	F	128	LEU	7.7
1	A	93	TYR	6.8
1	D	99	LEU	6.7
1	F	131	SER	6.3
1	F	129	GLY	5.6
1	F	132	SER	5.6
1	C	240	TRP	5.4
1	F	135	ALA	5.3
1	D	172	GLN	5.2
1	F	125	ALA	5.1
1	D	129	GLY	5.1
1	D	139	GLY	4.8
1	C	236	THR	4.8
1	C	234	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	96	GLU	4.7
1	D	170	LEU	4.4
1	F	126	GLN	4.3
1	F	137	MET	4.2
1	A	287	ALA	4.2
1	C	235	SER	4.1
1	D	168	VAL	4.1
1	F	102	ARG	4.0
1	D	169	GLN	4.0
1	F	175	LYS	4.0
1	D	98	GLN	4.0
1	D	171	GLY	3.6
1	F	136	SER	3.6
1	D	130	LEU	3.5
1	A	235	SER	3.5
1	F	121	ILE	3.3
1	F	122	ALA	3.3
1	D	167	LEU	3.3
1	C	95	SER	3.3
1	D	137	MET	3.3
1	E	217	LEU	3.3
1	C	233	ASP	3.1
1	D	282	ASN	3.1
1	D	163	GLU	3.1
1	E	213	ILE	3.0
1	D	173	ALA	2.9
1	F	123	GLU	2.9
1	F	109	GLU	2.9
1	B	246	MET	2.8
1	A	217	LEU	2.8
1	D	162	GLU	2.8
1	D	174	GLU	2.8
1	B	134	ALA	2.8
1	F	107	ALA	2.7
1	D	97	GLU	2.7
1	E	218	SER	2.7
1	B	98	GLN	2.7
1	D	102	ARG	2.7
1	C	238	PHE	2.6
1	E	220	LEU	2.6
1	C	232	GLY	2.6
1	C	281	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	138	PHE	2.6
1	D	237	ASP	2.6
1	D	166	LYS	2.6
1	D	249	ALA	2.6
1	A	213	ILE	2.6
1	F	100	GLN	2.5
1	C	177	LYS	2.5
1	D	103	ILE	2.5
1	F	106	ALA	2.5
1	E	241	TYR	2.5
1	B	217	LEU	2.4
1	C	282	ASN	2.4
1	E	248	ALA	2.4
1	C	271	ARG	2.4
1	B	99	LEU	2.4
1	E	216	SER	2.4
1	B	241	TYR	2.4
1	F	167	LEU	2.4
1	D	253	THR	2.4
1	E	221	THR	2.4
1	E	99	LEU	2.3
1	D	236	THR	2.3
1	F	124	GLY	2.3
1	D	100	GLN	2.3
1	F	282	ASN	2.3
1	B	96	GLU	2.3
1	F	240	TRP	2.3
1	F	103	ILE	2.3
1	C	237	ASP	2.3
1	E	246[A]	MET	2.2
1	E	214	PRO	2.2
1	A	208	MET	2.2
1	B	208	MET	2.2
1	C	226[A]	ASP	2.1
1	F	127	SER	2.1
1	D	234	GLN	2.1
1	E	234	GLN	2.1
1	E	252	ASN	2.1
1	B	213	ILE	2.1
1	D	95	SER	2.1
1	F	264	PRO	2.1
1	D	256	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	97	GLU	2.1
1	D	252	ASN	2.1
1	E	97	GLU	2.1
1	D	133	ALA	2.0
1	F	110	PHE	2.0
1	D	159	ARG	2.0
1	D	208[A]	MET	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	301	5/5	0.70	0.27	138,156,173,183	0
3	64Z	B	302	11/11	0.71	0.46	80,103,127,131	0
5	FOF	A	304	16/16	0.79	0.53	82,111,132,133	0
3	64Z	D	302	11/11	0.84	0.47	72,90,128,128	0
4	N1S	A	303	16/16	0.84	0.51	70,104,142,171	0
3	64Z	A	302	11/11	0.88	0.37	78,97,118,118	0
6	FOH	D	303	16/16	0.89	0.45	47,85,124,133	0
2	SO4	E	301	5/5	0.91	0.23	125,126,138,149	0
2	SO4	D	301	5/5	0.92	0.31	131,136,141,151	0
2	SO4	F	301	5/5	0.93	0.21	149,152,165,168	0
2	SO4	A	301	5/5	0.96	0.11	95,101,116,132	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.