



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:17 AM UTC

PDB ID : 6DEW / pdb\_00006dew  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

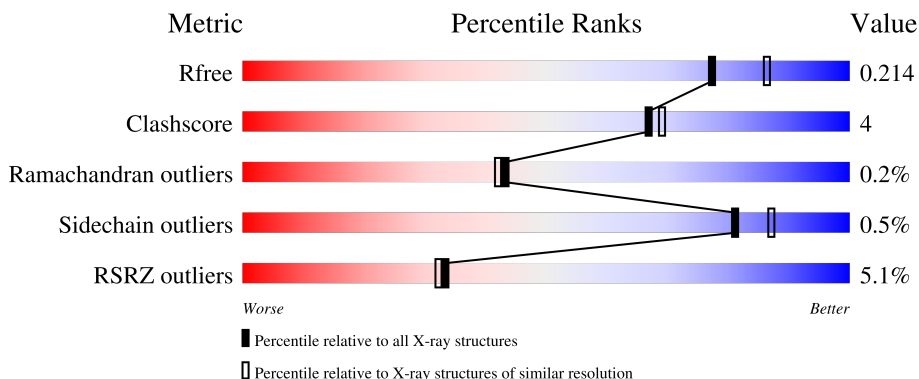
# 1 Overall quality at a glance

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.



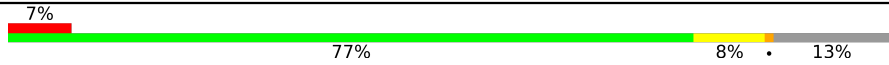
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of 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	 2% 85% 6% 8%
1	B	212	 3% 86% 10%
1	C	212	 3% 79% 9% 11%
1	D	212	 8% 82% 7% 11%
1	E	212	 4% 84% 6% 10%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	212	 <p>7% 77% 8% 13%</p>

## 2 Entry composition [i](#)

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

There are 18 discrepancies between the modelled and reference sequences:

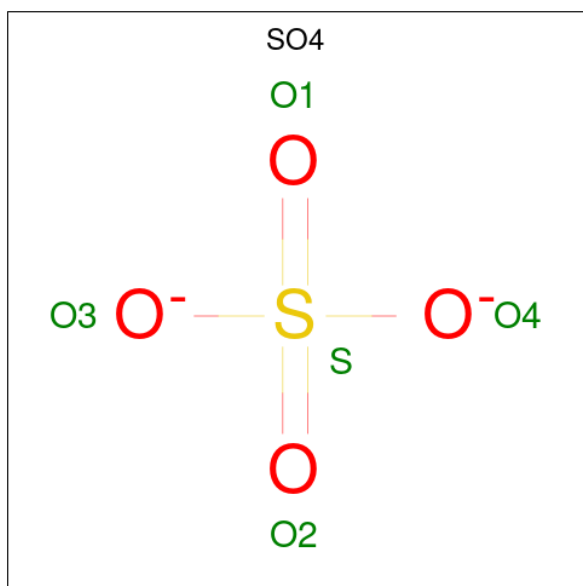
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	SER	-	expression tag	UNP O75208
A	77	HIS	-	expression tag	UNP O75208
A	78	MET	-	expression tag	UNP O75208
B	76	SER	-	expression tag	UNP O75208
B	77	HIS	-	expression tag	UNP O75208
B	78	MET	-	expression tag	UNP O75208
C	76	SER	-	expression tag	UNP O75208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

*Continued on next page...*

Continued from previous page...

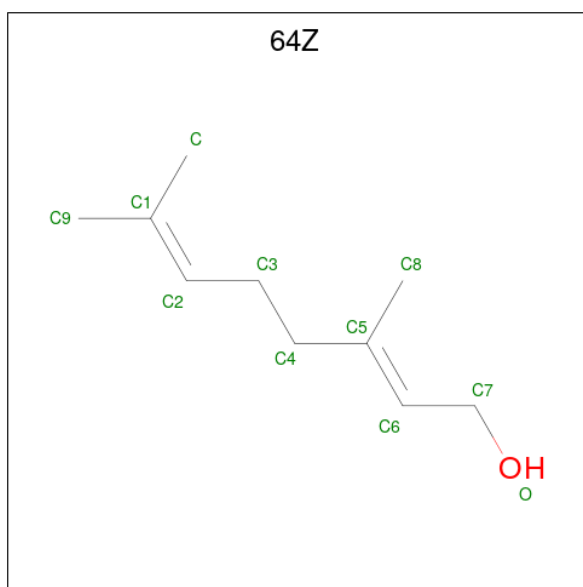
Chain	Residue	Modelled	Actual	Comment	Reference
F	78	MET	-	expression tag	UNP O75208

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



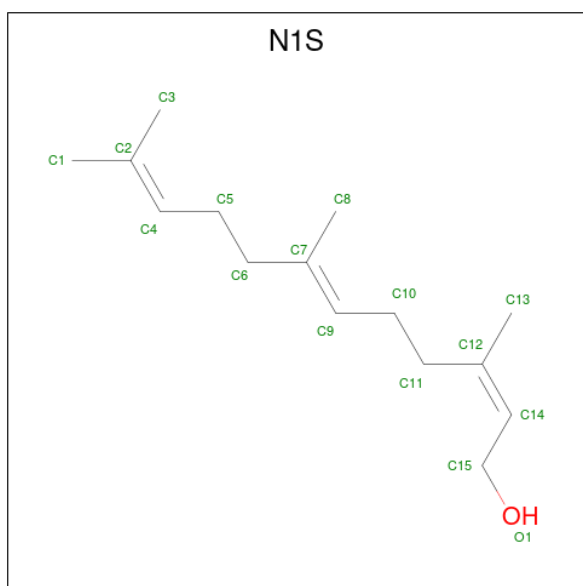
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

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



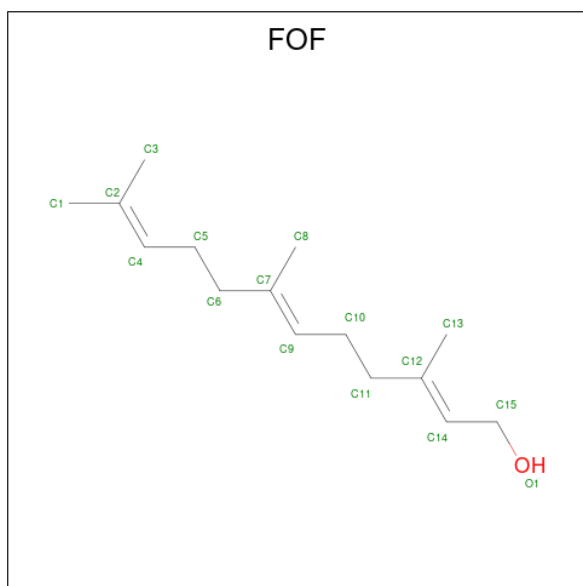
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	29	10	18	1	0	0
3	B	1	29	10	18	1	0	0
3	D	1	29	10	18	1	0	0

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



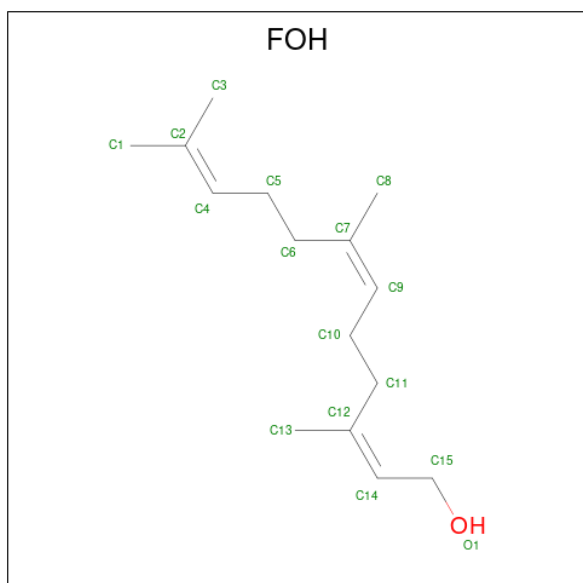
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	42	15	26	1	0	0

- Molecule 5 is (2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-ol (CCD ID: FOF) (formula: C<sub>15</sub>H<sub>26</sub>O).



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

- Molecule 6 is (2Z,6Z)-3,7,11-trimethyldodeca-2,6,10-trien-1-ol (CCD ID: FOH) (formula: C<sub>15</sub>H<sub>26</sub>O).



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

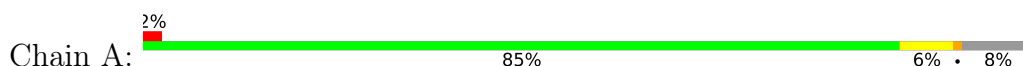
- Molecule 7 is water.

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		

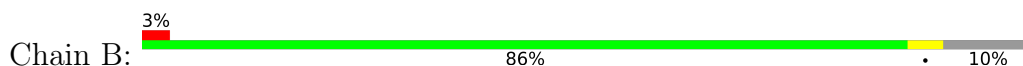
### 3 Residue-property plots [i](#)

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.

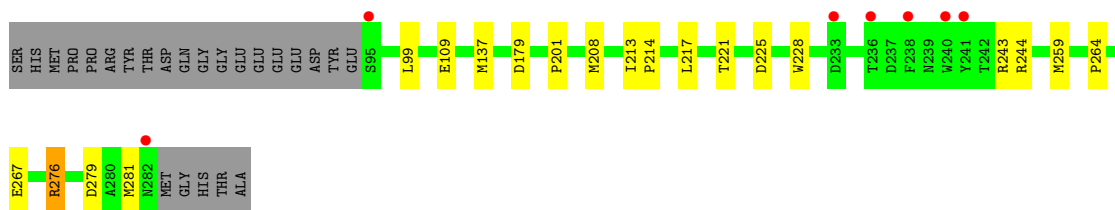
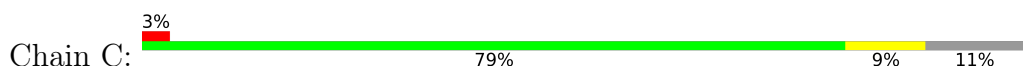
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



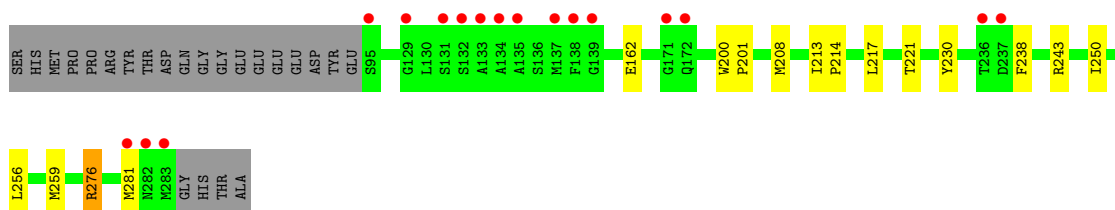
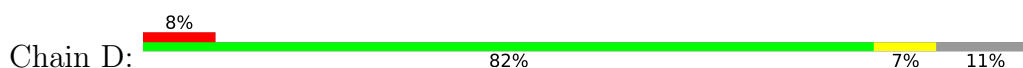
- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



- Molecule 1: Ubiquinone biosynthesis protein COQ9, mitochondrial



## 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) 93.0 (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)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.169 , 0.209 0.177 , 0.214	Depositor DCC
$R_{free}$ test set	2045 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage'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: SO4, FOF, FOH, N1S, 64Z

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	1.01	3/1607 (0.2%)	0.90	0/2177
1	B	0.99	3/1573 (0.2%)	0.88	0/2133
1	C	0.90	1/1556 (0.1%)	0.82	0/2111
1	D	0.76	0/1557	0.74	0/2110
1	E	0.95	1/1569 (0.1%)	0.83	0/2127
1	F	0.78	1/1516 (0.1%)	0.73	0/2055
All	All	0.90	9/9378 (0.1%)	0.82	0/12713

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	111	VAL	CA-CB	7.29	1.58	1.54
1	B	259	MET	SD-CE	-7.24	1.61	1.79
1	B	194	ILE	CA-CB	7.09	1.58	1.54
1	A	259	MET	CB-CG	6.60	1.72	1.52
1	C	208	MET	CB-CG	6.22	1.71	1.52
1	A	223	MET	CG-SD	-5.39	1.67	1.80
1	B	111	VAL	CA-CB	-5.27	1.51	1.54
1	A	150	VAL	CB-CG1	5.19	1.69	1.52
1	E	243	ARG	CB-CG	-5.08	1.37	1.52

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	1573	1522	1521	10	0
1	B	1540	1493	1491	12	0
1	C	1524	1478	1476	11	0
1	D	1525	1485	1484	12	0
1	E	1536	1496	1495	19	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
5	A	16	26	0	0	0
6	D	16	26	26	2	0
7	A	93	0	0	1	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	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (67) 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:E:242:THR:HG22	1:E:246[B]:MET:HE3	1.59	0.84
1:D:208[B]:MET:HE1	6:D:303:FOH:C4	2.14	0.77
1:B:246:MET:HG2	1:E:246[B]:MET:HG2	1.67	0.76
1:E:242:THR:CG2	1:E:246[B]:MET:HE3	2.15	0.76
1:B:246:MET:SD	1:E:246[B]:MET:HE2	2.25	0.76
1:E:246[A]:MET:HE1	1:E:281:MET:HE1	1.68	0.75
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:246[A]:MET:HE1	1:A:281:MET:HE1	1.82	0.62
1:B:246:MET:CG	1:E:246[B]:MET:HE2	2.31	0.61
1:B:246:MET:HE1	1:E:283:MET:HG2	1.83	0.60
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:A:246[A]:MET:CE	1:A:281:MET:HE1	2.35	0.56
1:E:246[A]:MET:CE	1:E:281:MET:HE1	2.36	0.55
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:D:208[B]:MET:HE1	6:D:303:FOH:C2	2.38	0.52
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: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:F:127:SER:C	1:F:128:LEU:HD23	2.37	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:A:166:LYS:NZ	7:A:404:HOH:O	2.46	0.48
1:C:201:PRO:HG3	1:C:259:MET:HE2	1.95	0.47
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:C:99:LEU:HD23	1:C:137:MET:HE1	1.96	0.46
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: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:D:281:MET:HA	1:D:281:MET:HE2	1.99	0.45
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:F:213:ILE:HG23	1:F:214:PRO:HD3	2.00	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:246:MET:HG2	1:E:246[B]:MET:HE2	2.00	0.42
1:C:109:GLU:HG3	7:C:346:HOH:O	2.19	0.42
1:E:246[A]:MET:CE	1:E:281:MET:CE	2.97	0.42
1:A:259:MET:HE3	1:A:259:MET:HB2	1.89	0.42
1:C:264:PRO:O	1:C:267:GLU:HG3	2.20	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:280:ALA:HA	1:E:283:MET:HE2	2.01	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:HD3	1:D:276:ARG:HA	1.81	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:A:234:GLN:O	1:A:235:SER:C	2.63	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%)	24	21
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%)	24	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1133/1272 (89%)	1107 (98%)	24 (2%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

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

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/183 (92%)	169 (100%)	0	100	100
1	B	166/183 (91%)	166 (100%)	0	100	100
1	C	165/183 (90%)	164 (99%)	1 (1%)	78	85
1	D	165/183 (90%)	164 (99%)	1 (1%)	78	85
1	E	165/183 (90%)	165 (100%)	0	100	100
1	F	160/183 (87%)	157 (98%)	3 (2%)	50	56
All	All	990/1098 (90%)	985 (100%)	5 (0%)	81	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	276	ARG
1	D	276	ARG
1	F	127	SER
1	F	226	ASP
1	F	276	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	252	ASN
1	B	114	HIS
1	B	282	ASN
1	D	152	GLN
1	F	148	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 oligosaccharides 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	$\# Z  > 2$
2	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.16	0
3	64Z	A	302	-	10,10,10	0.86	0	11,11,11	1.60	3 (27%)
6	FOH	D	303	-	15,15,15	0.87	1 (6%)	17,17,17	1.65	4 (23%)
2	SO4	F	301	-	4,4,4	0.25	0	6,6,6	0.09	0
3	64Z	D	302	-	10,10,10	1.13	0	11,11,11	1.98	5 (45%)
2	SO4	E	301	-	4,4,4	0.22	0	6,6,6	0.20	0
5	FOF	A	304	-	15,15,15	0.72	0	17,17,17	1.69	4 (23%)
2	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	64Z	B	302	-	10,10,10	0.85	0	11,11,11	1.81	3 (27%)
4	N1S	A	303	-	15,15,15	0.75	0	17,17,17	1.41	3 (17%)
2	SO4	A	301	-	4,4,4	0.22	0	6,6,6	0.25	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	64Z	A	302	-	-	1/9/9/9	-
6	FOH	D	303	-	-	4/15/15/15	-
3	64Z	D	302	-	-	4/9/9/9	-
5	FOF	A	304	-	-	3/15/15/15	-
3	64Z	B	302	-	-	3/9/9/9	-
4	N1S	A	303	-	-	5/15/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	303	FOH	C13-C12	2.15	1.55	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	64Z	C8-C5-C4	4.49	123.02	115.23
5	A	304	FOF	C10-C9-C7	-3.97	118.53	127.62
3	B	302	64Z	C8-C5-C4	3.61	121.49	115.23
6	D	303	FOH	C13-C12-C11	3.28	120.92	115.23
6	D	303	FOH	C8-C7-C6	3.09	120.59	115.23
6	D	303	FOH	C8-C7-C9	-3.08	115.73	123.63
5	A	304	FOF	C13-C12-C11	2.89	120.24	115.23
3	A	302	64Z	C8-C5-C4	2.86	120.20	115.23
4	A	303	N1S	C13-C12-C11	2.79	120.07	115.23
5	A	304	FOF	C11-C12-C14	-2.51	115.52	121.17
4	A	303	N1S	C10-C9-C7	-2.51	121.88	127.62
3	B	302	64Z	C-C1-C9	2.48	120.30	114.59
6	D	303	FOH	C5-C4-C2	-2.41	119.62	127.64
4	A	303	N1S	C13-C12-C14	-2.40	117.45	123.63
3	A	302	64Z	C-C1-C9	2.37	120.04	114.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304	FOF	C8-C7-C6	2.34	119.30	115.23
3	D	302	64Z	C-C1-C9	2.21	119.67	114.59
3	D	302	64Z	C4-C5-C6	-2.19	116.24	121.17
3	D	302	64Z	C3-C2-C1	-2.13	120.52	127.64
3	D	302	64Z	C7-C6-C5	-2.09	119.43	126.38
3	B	302	64Z	C3-C2-C1	-2.08	120.70	127.64
3	A	302	64Z	C3-C2-C1	-2.05	120.82	127.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	303	FOH	2	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%)	-0.02	5 (2%) 57 56	21, 44, 83, 117	1 (0%)
1	B	191/212 (90%)	0.05	6 (3%) 51 50	20, 47, 82, 108	1 (0%)
1	C	188/212 (88%)	0.13	7 (3%) 45 44	21, 49, 88, 108	2 (1%)
1	D	189/212 (89%)	0.46	17 (8%) 15 14	21, 58, 117, 145	1 (0%)
1	E	191/212 (90%)	0.12	9 (4%) 36 35	24, 47, 93, 122	1 (0%)
1	F	184/212 (86%)	0.45	14 (7%) 20 18	20, 60, 122, 150	1 (0%)
All	All	1138/1272 (89%)	0.19	58 (5%) 33 32	20, 51, 101, 150	7 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	PHE	4.9
1	D	283	MET	4.4
1	F	283	MET	4.2
1	D	133	ALA	4.1
1	E	287	ALA	4.0
1	A	287	ALA	3.7
1	C	240	TRP	3.7
1	C	95	SER	3.6
1	B	246	MET	3.5
1	D	129	GLY	3.3
1	F	133	ALA	3.3
1	D	132	SER	3.3
1	F	282	ASN	3.2
1	D	139	GLY	3.2
1	A	235	SER	3.1
1	F	236	THR	3.0
1	A	286	THR	3.0
1	F	134	ALA	3.0
1	B	235	SER	3.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	285	HIS	3.0
1	E	134	ALA	2.9
1	F	135	ALA	2.9
1	C	236	THR	2.9
1	D	137	MET	2.9
1	C	241	TYR	2.9
1	D	172	GLN	2.8
1	D	236	THR	2.8
1	D	282	ASN	2.8
1	E	232	GLY	2.8
1	D	134	ALA	2.8
1	D	135	ALA	2.8
1	E	233	ASP	2.7
1	A	93	TYR	2.7
1	C	282	ASN	2.7
1	E	234	GLN	2.7
1	A	285	HIS	2.7
1	F	175	LYS	2.7
1	D	237	ASP	2.6
1	F	240	TRP	2.6
1	F	128	LEU	2.6
1	B	233	ASP	2.5
1	B	286	THR	2.5
1	E	130	LEU	2.5
1	B	284	GLY	2.5
1	B	285	HIS	2.5
1	E	231	ALA	2.5
1	D	95	SER	2.4
1	C	233	ASP	2.4
1	D	171	GLY	2.3
1	C	238	PHE	2.3
1	F	130	LEU	2.2
1	F	241	TYR	2.2
1	F	126	GLN	2.2
1	F	107	ALA	2.1
1	D	281	MET	2.1
1	E	97	GLU	2.1
1	F	129	GLY	2.1
1	D	131	SER	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 oligosaccharides 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	F	301	5/5	0.60	0.16	149,152,165,168	0
2	SO4	B	301	5/5	0.69	0.21	138,156,173,183	0
2	SO4	E	301	5/5	0.78	0.18	125,126,138,149	0
2	SO4	D	301	5/5	0.79	0.20	131,136,141,151	0
3	64Z	B	302	11/11	0.80	0.37	80,103,127,131	0
2	SO4	A	301	5/5	0.83	0.11	95,101,116,132	0
5	FOF	A	304	16/16	0.84	0.31	82,111,132,133	0
4	N1S	A	303	16/16	0.86	0.33	70,104,142,171	0
3	64Z	D	302	11/11	0.88	0.26	72,90,128,128	0
3	64Z	A	302	11/11	0.90	0.20	78,97,118,118	0
6	FOH	D	303	16/16	0.90	0.21	47,85,124,133	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.