



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2019 – 08:09 PM EDT

PDB ID : 2CB2  
Title : Sulfur Oxygenase Reductase from Acidianus Ambivalens  
Authors : Urich, T.; Gomes, C.M.; Kletzin, A.; Frazao, C.  
Deposited on : 2005-12-28  
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

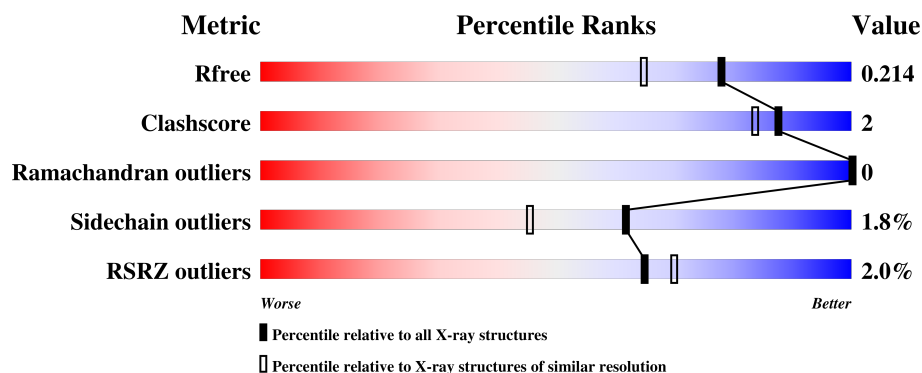
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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	318	 88% 8% . .
1	B	318	 87% 9% .
1	C	318	 89% 7% . .
1	D	318	 88% 8% .
1	E	318	 87% 9% .

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	318	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>86%</div><div>10%</div><div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15520 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 SULFUR OXYGENASE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	12	0
			2517	1632	413	448	24			
1	B	307	Total	C	N	O	S	0	9	0
			2500	1618	413	447	22			
1	C	307	Total	C	N	O	S	0	8	0
			2499	1620	412	446	21			
1	D	307	Total	C	N	O	S	0	10	0
			2510	1628	411	448	23			
1	E	307	Total	C	N	O	S	0	8	0
			2500	1620	410	447	23			
1	F	307	Total	C	N	O	S	0	12	0
			2511	1629	412	448	22			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

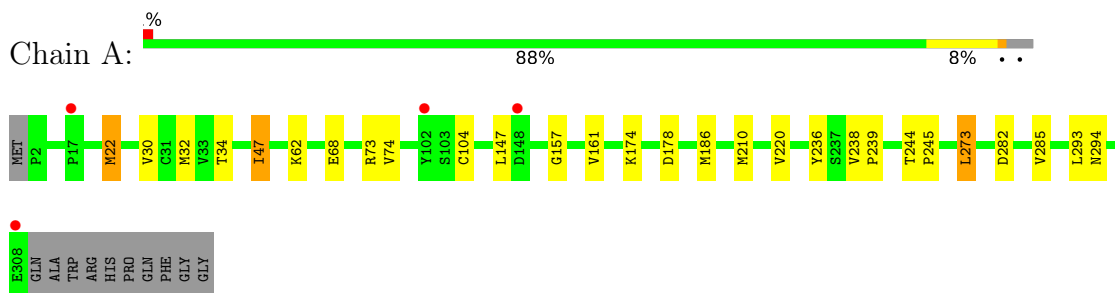
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total 80	O 80	0	0
3	B	81	Total 81	O 81	0	0
3	C	82	Total 82	O 82	0	0
3	D	78	Total 78	O 78	0	0
3	E	70	Total 70	O 70	0	0
3	F	86	Total 86	O 86	0	0

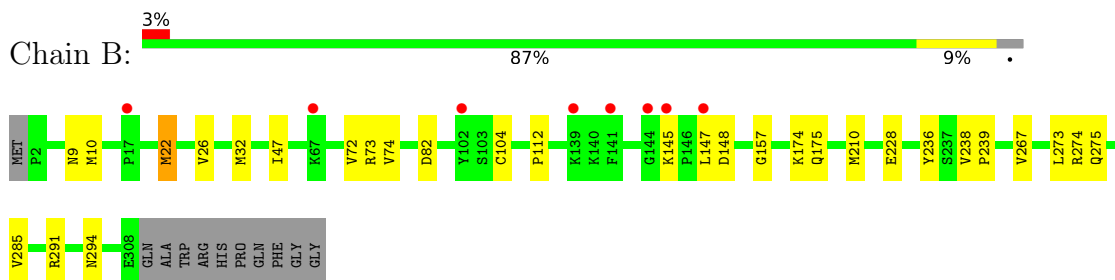
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

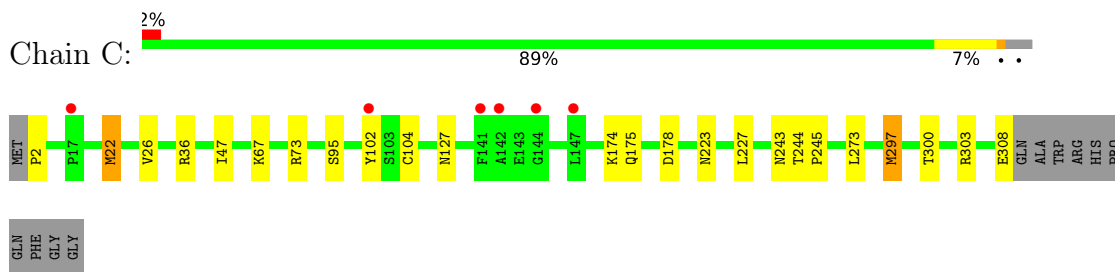
#### • Molecule 1: SULFUR OXYGENASE REDUCTASE



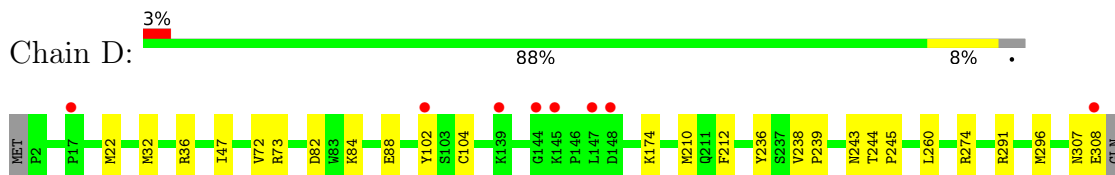
#### • Molecule 1: SULFUR OXYGENASE REDUCTASE



#### • Molecule 1: SULFUR OXYGENASE REDUCTASE

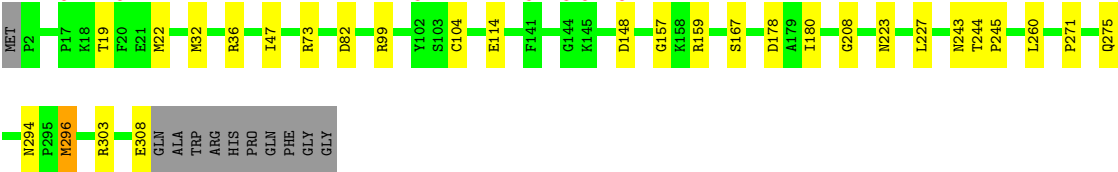
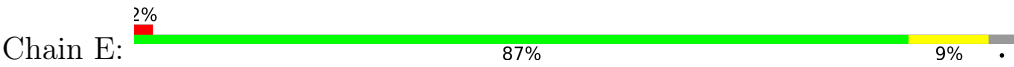


#### • Molecule 1: SULFUR OXYGENASE REDUCTASE

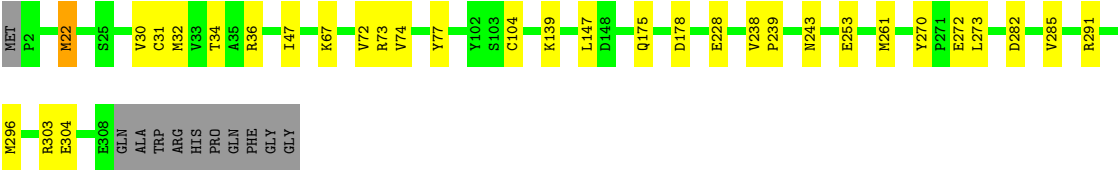
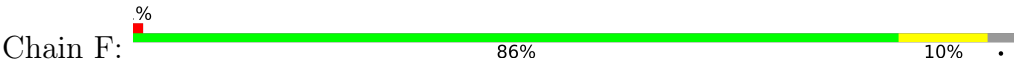


ALA  
TRP  
ARG  
HIS  
PRO  
GLN  
PHE  
GLY

• Molecule 1: SULFUR OXYGENASE REDUCTASE



• Molecule 1: SULFUR OXYGENASE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.15Å 162.15Å 154.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.80 – 1.70 49.21 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (111.80-1.70) 99.8 (49.21-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.183 , 0.210 0.192 , 0.214	Depositor DCC
$R_{free}$ test set	1288 reflections (0.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -l,-k,-h 0.000 for -h,-l,-k 0.000 for -h,l,k 0.004 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CSS

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	0.92	1/2631 (0.0%)	0.91	6/3563 (0.2%)
1	B	0.94	1/2601 (0.0%)	0.94	7/3523 (0.2%)
1	C	0.92	1/2600 (0.0%)	0.95	8/3523 (0.2%)
1	D	0.95	1/2615 (0.0%)	0.90	5/3542 (0.1%)
1	E	0.98	2/2597 (0.1%)	0.95	11/3518 (0.3%)
1	F	0.93	4/2628 (0.2%)	0.95	10/3561 (0.3%)
All	All	0.94	10/15672 (0.1%)	0.93	47/21230 (0.2%)

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
1	D	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	167	SER	CB-OG	-7.11	1.33	1.42
1	F	304	GLU	CD-OE2	-6.18	1.18	1.25
1	A	32	MET	SD-CE	-5.86	1.45	1.77
1	F	175	GLN	CD-NE2	5.69	1.47	1.32
1	E	32	MET	SD-CE	-5.59	1.46	1.77
1	F	32	MET	SD-CE	-5.52	1.47	1.77
1	B	175	GLN	CB-CG	5.37	1.67	1.52
1	C	175	GLN	CD-NE2	5.33	1.46	1.32
1	D	32	MET	SD-CE	-5.11	1.49	1.77
1	F	253	GLU	CD-OE1	-5.08	1.20	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	ASP	CB-CG-OD1	8.45	125.91	118.30
1	E	178[A]	ASP	CB-CG-OD2	8.41	125.87	118.30
1	E	178[B]	ASP	CB-CG-OD2	8.41	125.87	118.30
1	E	82	ASP	CB-CG-OD1	8.39	125.85	118.30
1	F	178[A]	ASP	CB-CG-OD2	7.53	125.08	118.30
1	F	178[B]	ASP	CB-CG-OD2	7.53	125.08	118.30
1	B	210	MET	CG-SD-CE	-7.38	88.40	100.20
1	F	36	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	C	73	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	D	73	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	36	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	32	MET	CG-SD-CE	6.91	111.26	100.20
1	E	73	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	F	36	ARG	NE-CZ-NH1	-6.69	116.96	120.30
1	C	36	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	178[A]	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	178[B]	ASP	CB-CG-OD2	6.39	124.05	118.30
1	C	303	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	B	148	ASP	CB-CG-OD2	6.32	123.98	118.30
1	C	73	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	73	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	273	LEU	CB-CG-CD1	6.23	121.59	111.00
1	C	178[A]	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	178[B]	ASP	CB-CG-OD2	6.19	123.87	118.30
1	E	36	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	E	36	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	273	LEU	CB-CG-CD1	5.91	121.05	111.00
1	E	73	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	73	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	282	ASP	CB-CG-OD1	5.75	123.47	118.30
1	F	73	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	E	303	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	F	273	LEU	CB-CG-CD1	5.65	120.61	111.00
1	A	73	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	73	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	274	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	F	291	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	F	303	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	82	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	291	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	E	99	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	297	MET	CG-SD-CE	5.21	108.53	100.20
1	F	303	ARG	NE-CZ-NH2	5.14	122.87	120.30

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	E	159	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	148	ASP	CB-CG-OD2	5.08	122.87	118.30
1	F	282	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	307	ASN	Peptide

## 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	2517	0	2475	12	0
1	B	2500	0	2454	11	0
1	C	2499	0	2454	9	0
1	D	2510	0	2464	14	0
1	E	2500	0	2451	11	0
1	F	2511	0	2468	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	80	0	0	0	0
3	B	81	0	0	0	0
3	C	82	0	0	0	0
3	D	78	0	0	0	0
3	E	70	0	0	0	0
3	F	86	0	0	0	0
All	All	15520	0	14766	66	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 2.

All (66) 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:F:261:MET:CE	1:F:261:MET:SD	2.03	1.47
1:B:10:MET:SD	1:B:10:MET:CE	2.01	1.46
1:C:297:MET:CE	1:C:297:MET:SD	2.03	1.45
1:D:22[B]:MET:SD	1:D:104:CYS:SG	2.72	0.87
1:A:22[A]:MET:SD	1:A:104:CYS:SG	2.79	0.79
1:F:30:VAL:O	1:F:34[A]:THR:HG23	1.82	0.79
1:D:210[A]:MET:HE3	1:D:212:PHE:HE2	1.53	0.72
1:B:22[A]:MET:SD	1:B:104:CYS:SG	2.93	0.64
1:E:22[B]:MET:SD	1:E:104:CYS:SG	2.98	0.60
1:D:84:LYS:O	1:D:88[B]:GLU:HG3	2.08	0.53
1:E:223:ASN:ND2	1:E:227:LEU:O	2.41	0.52
1:F:30:VAL:O	1:F:34[B]:THR:HG22	2.08	0.52
1:D:210[A]:MET:CE	1:D:212:PHE:HE2	2.22	0.52
1:E:271:PRO:O	1:E:275:GLN:HG2	2.10	0.51
1:C:223:ASN:ND2	1:C:227:LEU:O	2.37	0.50
1:E:19:THR:O	1:E:22[B]:MET:HG3	2.12	0.50
1:C:22:MET:SD	1:C:104:CYS:SG	3.06	0.49
1:A:30:VAL:O	1:A:34[B]:THR:HG23	2.12	0.49
1:D:47[B]:ILE:HD13	1:D:296:MET:SD	2.53	0.49
1:D:244:THR:HA	1:D:245:PRO:C	2.34	0.48
1:F:22:MET:SD	1:F:104:CYS:SG	3.11	0.48
1:D:22[B]:MET:CE	1:D:104:CYS:SG	3.03	0.47
1:D:243[A]:ASN:OD1	1:F:243[A]:ASN:ND2	2.32	0.47
1:C:2:PRO:HD3	1:C:308:GLU:HG3	1.97	0.47
1:F:47[A]:ILE:CD1	1:F:74:VAL:HG12	2.45	0.46
1:A:210[B]:MET:HE1	1:A:220:VAL:HG22	1.98	0.45
1:C:243[A]:ASN:ND2	1:E:243[A]:ASN:OD1	2.37	0.45
1:D:236:TYR:CE2	1:F:285:VAL:HA	2.52	0.45
1:A:47[B]:ILE:HG13	1:A:74:VAL:HG12	1.99	0.44
1:B:47[B]:ILE:HG22	1:B:74:VAL:HG12	1.98	0.44
1:F:31:CSS:HA	1:F:34[B]:THR:CG2	2.47	0.44
1:A:157:GLY:HA2	1:A:294:ASN:OD1	2.17	0.44
1:F:47[B]:ILE:HG12	1:F:296:MET:SD	2.57	0.44
1:F:47[A]:ILE:HG23	1:F:72:VAL:CG2	2.48	0.44
1:B:157:GLY:HA2	1:B:294:ASN:OD1	2.18	0.44
1:E:157:GLY:HA2	1:E:294:ASN:OD1	2.18	0.44
1:F:31:CSS:HA	1:F:34[B]:THR:HG22	2.00	0.44
1:F:270:TYR:CE2	1:F:272:GLU:HG2	2.52	0.44
1:E:244:THR:HA	1:E:245:PRO:C	2.39	0.43
1:E:260:LEU:C	1:E:260:LEU:HD23	2.39	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:MET:CE	1:F:261:MET:CG	2.94	0.43
1:A:238:VAL:HB	1:A:239:PRO:HD3	2.00	0.43
1:B:267:VAL:O	1:B:274:ARG:HA	2.18	0.43
1:B:267:VAL:HA	1:B:273:LEU:HG	2.00	0.43
1:F:238:VAL:HB	1:F:239:PRO:HD3	1.99	0.43
1:A:244:THR:HA	1:A:245:PRO:C	2.39	0.43
1:C:297:MET:CE	1:C:297:MET:HB3	2.48	0.43
1:C:244:THR:HA	1:C:245:PRO:C	2.39	0.42
1:D:260:LEU:HD23	1:D:260:LEU:C	2.40	0.42
1:A:236:TYR:CE2	1:B:285:VAL:HA	2.54	0.42
1:D:47[B]:ILE:HG23	1:D:72:VAL:CG2	2.49	0.42
1:B:238:VAL:HB	1:B:239:PRO:HD3	2.02	0.41
1:D:238:VAL:HB	1:D:239:PRO:HD3	2.01	0.41
1:E:47:ILE:HG12	1:E:296:MET:SD	2.61	0.41
1:A:285:VAL:HA	1:B:236:TYR:CE2	2.56	0.41
1:A:186:MET:HB2	1:A:273:LEU:HD13	2.01	0.41
1:A:161:VAL:HB	1:A:293:LEU:HB2	2.02	0.41
1:B:9:ASN:HD21	1:B:112:PRO:HB2	1.85	0.41
1:E:114:GLU:OE1	1:E:208:GLY:HA3	2.21	0.41
1:C:127:ASN:HD22	1:C:300:THR:HB	1.86	0.40
1:E:180:ILE:HA	1:E:180:ILE:HD12	1.99	0.40
1:B:47[A]:ILE:HG23	1:B:72:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/318 (99%)	308 (98%)	8 (2%)	0	100	100
1	B	313/318 (98%)	307 (98%)	6 (2%)	0	100	100
1	C	312/318 (98%)	305 (98%)	7 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	314/318 (99%)	306 (98%)	8 (2%)	0	100	100
1	E	312/318 (98%)	306 (98%)	6 (2%)	0	100	100
1	F	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
All	All	1883/1908 (99%)	1842 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	276/272 (102%)	268 (97%)	8 (3%)	45	25
1	B	273/272 (100%)	265 (97%)	8 (3%)	45	25
1	C	272/272 (100%)	265 (97%)	7 (3%)	49	30
1	D	274/272 (101%)	272 (99%)	2 (1%)	85	79
1	E	272/272 (100%)	270 (99%)	2 (1%)	85	79
1	F	276/272 (102%)	270 (98%)	6 (2%)	55	36
All	All	1643/1632 (101%)	1610 (98%)	33 (2%)	62	40

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	MET
1	A	22[B]	MET
1	A	47[A]	ILE
1	A	47[B]	ILE
1	A	62	LYS
1	A	68	GLU
1	A	147	LEU
1	A	174	LYS
1	B	22[A]	MET
1	B	22[B]	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	26	VAL
1	B	145	LYS
1	B	147	LEU
1	B	174	LYS
1	B	228	GLU
1	B	275	GLN
1	C	22	MET
1	C	26	VAL
1	C	47[A]	ILE
1	C	47[B]	ILE
1	C	67	LYS
1	C	95	SER
1	C	174	LYS
1	D	174	LYS
1	D	308	GLU
1	E	296	MET
1	E	308	GLU
1	F	22	MET
1	F	67	LYS
1	F	77	TYR
1	F	139	LYS
1	F	147	LEU
1	F	228	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	127	ASN
1	A	247	GLN
1	A	307	ASN
1	B	9	ASN
1	B	247	GLN
1	C	127	ASN
1	C	247	GLN
1	C	307	ASN
1	D	45	ASN
1	D	127	ASN
1	D	247	GLN
1	D	275	GLN
1	E	127	ASN
1	E	247	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	247	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	CSS	A	31	1	5,6,7	0.68	0	2,6,8	0.95	0
1	CSS	B	31	1	5,6,7	0.88	0	2,6,8	1.19	0
1	CSS	C	31	1	5,6,7	0.33	0	2,6,8	1.62	1 (50%)
1	CSS	D	31	1	5,6,7	0.71	0	2,6,8	0.98	0
1	CSS	E	31	1	5,6,7	0.80	0	2,6,8	1.64	1 (50%)
1	CSS	F	31	1	5,6,7	1.13	0	2,6,8	1.00	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
1	CSS	A	31	1	-	0/1/5/7	-
1	CSS	B	31	1	-	0/1/5/7	-
1	CSS	C	31	1	-	0/1/5/7	-
1	CSS	D	31	1	-	0/1/5/7	-
1	CSS	E	31	1	-	0/1/5/7	-
1	CSS	F	31	1	-	0/1/5/7	-

There are no bond length outliers.



All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	31	CSS	O-C-CA	-2.32	118.75	124.98
1	C	31	CSS	O-C-CA	-2.24	118.97	124.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	31	CSS	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	306/318 (96%)	-0.25	4 (1%)	77 81	25, 31, 46, 54	0
1	B	306/318 (96%)	-0.05	8 (2%)	56 61	26, 32, 47, 56	0
1	C	306/318 (96%)	-0.05	6 (1%)	65 70	25, 32, 48, 55	0
1	D	306/318 (96%)	-0.09	8 (2%)	56 61	26, 32, 48, 56	0
1	E	306/318 (96%)	-0.12	7 (2%)	60 65	26, 32, 48, 53	0
1	F	306/318 (96%)	-0.24	3 (0%)	82 85	25, 31, 46, 55	0
All	All	1836/1908 (96%)	-0.13	36 (1%)	65 70	25, 31, 48, 56	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	102[A]	TYR	4.6
1	E	102[A]	TYR	4.5
1	C	147	LEU	4.3
1	C	17	PRO	4.0
1	D	147	LEU	3.3
1	B	141	PHE	3.1
1	D	144	GLY	3.0
1	D	102[A]	TYR	2.9
1	E	17	PRO	2.9
1	A	102[A]	TYR	2.9
1	D	17	PRO	2.8
1	B	102	TYR	2.7
1	E	144	GLY	2.7
1	E	141	PHE	2.7
1	C	102[A]	TYR	2.6
1	B	147	LEU	2.6
1	E	145	LYS	2.6
1	A	308	GLU	2.5
1	B	145	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	139	LYS	2.5
1	D	148	ASP	2.4
1	A	148	ASP	2.3
1	B	67	LYS	2.3
1	D	145	LYS	2.3
1	F	25	SER	2.3
1	B	139	LYS	2.3
1	D	308	GLU	2.2
1	C	141	PHE	2.2
1	C	142	ALA	2.2
1	B	144	GLY	2.2
1	C	144	GLY	2.2
1	A	17	PRO	2.2
1	F	148	ASP	2.1
1	E	148	ASP	2.1
1	E	20	PHE	2.0
1	B	17	PRO	2.0

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

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
1	CSS	D	31	7/8	0.86	0.11	30,32,44,63	0
1	CSS	E	31	7/8	0.87	0.11	29,32,44,67	0
1	CSS	C	31	7/8	0.87	0.09	32,32,46,66	0
1	CSS	A	31	7/8	0.90	0.10	31,34,44,63	0
1	CSS	F	31	7/8	0.91	0.10	31,32,45,65	0
1	CSS	B	31	7/8	0.93	0.07	31,34,45,65	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
2	FE	B	1310	1/1	0.98	0.14	46,46,46,46	0
2	FE	F	1310	1/1	0.99	0.18	44,44,44,44	0
2	FE	D	1310	1/1	0.99	0.17	45,45,45,45	0
2	FE	E	1310	1/1	0.99	0.17	47,47,47,47	0
2	FE	A	1310	1/1	0.99	0.17	45,45,45,45	0
2	FE	C	1310	1/1	0.99	0.15	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.