



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TV7  
Title : Structure of the S-adenosylmethionine dependent Enzyme MoaA  
Authors : Haenzelmann, P.; Schindelin, H.  
Deposited on : 2004-06-28  
Resolution : 2.80 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

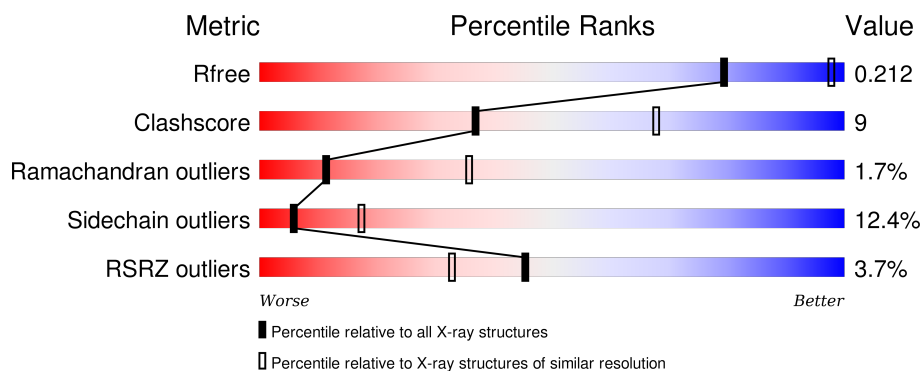
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

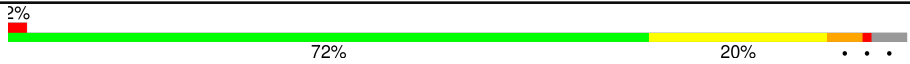

The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	340	
1	B	340	

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
2	SO4	A	1403	-	-	-	X
2	SO4	B	2403	-	-	X	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5379 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 Molybdenum cofactor biosynthesis protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2641	1673	455	500	13			
1	B	326	Total	C	N	O	S	0	0	0
			2632	1668	454	497	13			

- 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		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

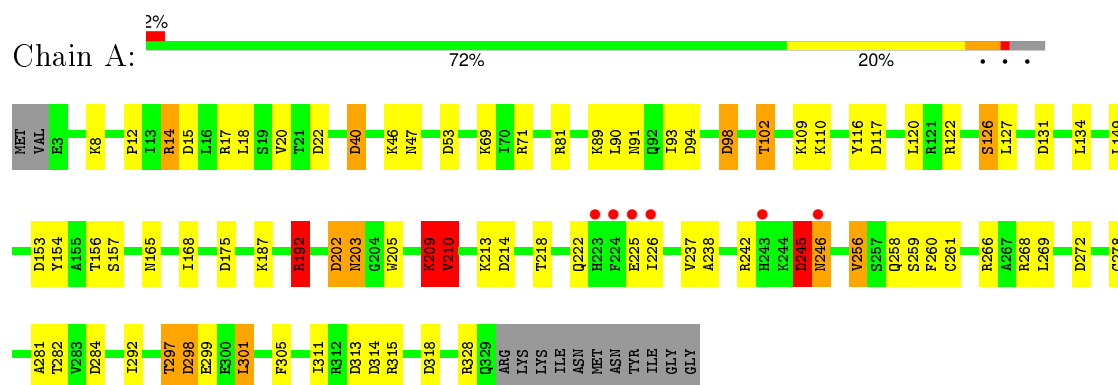
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	16	Total	O	0	0
			16	16		

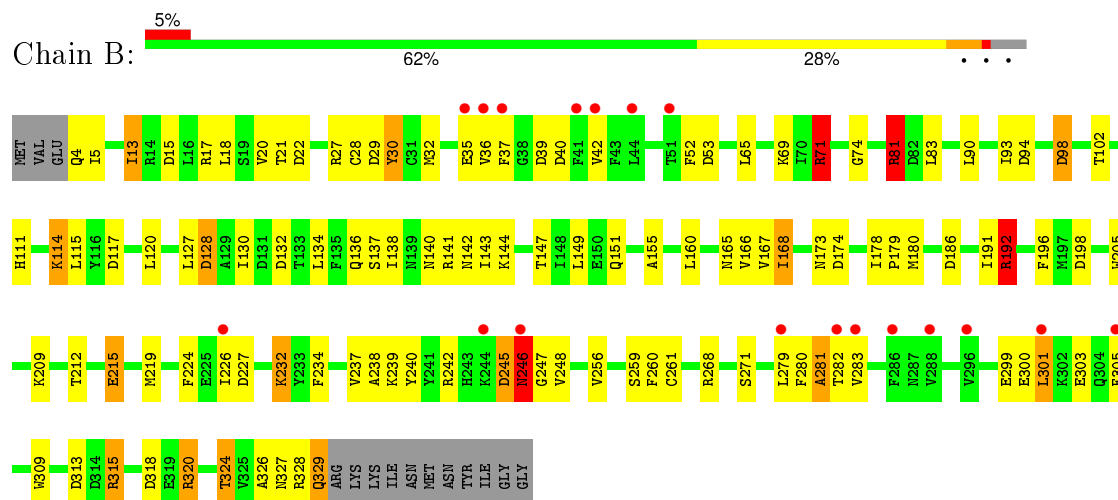
### 3 Residue-property plots

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: Molybdenum cofactor biosynthesis protein A



#### • Molecule 1: Molybdenum cofactor biosynthesis protein A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.12Å 102.44Å 191.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 49.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.80) 98.5 (49.47-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.28 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.187 , 0.211 0.198 , 0.212	Depositor DCC
$R_{free}$ test set	1213 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23771 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.375 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: SF4, 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	0.97	1/2684 (0.0%)	1.09	21/3613 (0.6%)
1	B	0.82	1/2675 (0.0%)	1.02	17/3601 (0.5%)
All	All	0.90	2/5359 (0.0%)	1.05	38/7214 (0.5%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	SER	CB-OG	-5.22	1.35	1.42
1	B	30	TYR	CD1-CE1	5.05	1.47	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ASP	CB-CG-OD2	9.38	126.74	118.30
1	B	313	ASP	CB-CG-OD2	8.30	125.77	118.30
1	B	29	ASP	CB-CG-OD2	7.93	125.44	118.30
1	A	313	ASP	CB-CG-OD2	7.68	125.22	118.30
1	B	40	ASP	CB-CG-OD2	7.21	124.79	118.30
1	B	192	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	175	ASP	CB-CG-OD2	7.19	124.77	118.30
1	B	94	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	209	LYS	C-N-CA	6.83	138.77	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	22	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	117	ASP	CB-CG-OD2	6.57	124.22	118.30
1	B	22	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	272	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	284	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	117	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	268	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	15	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	192	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	128	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	214	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	39	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	298	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	98	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	15	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	94	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	192	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	227	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	117	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	210	VAL	N-CA-C	5.42	125.65	111.00
1	B	71	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	131	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	209	LYS	CA-C-N	5.15	128.54	117.20
1	A	245	ASP	C-N-CA	5.15	134.57	121.70
1	A	245	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	98	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	268	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	186	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	GLY	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	2641	0	2637	41	0
1	B	2632	0	2631	61	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
4	A	48	0	0	2	0
4	B	16	0	0	4	0
All	All	5379	0	5268	99	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 9.

All (99) 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:219:MET:SD	1:B:219:MET:CE	2.04	1.46
1:A:245:ASP:HB2	1:A:246:ASN:HB3	1.44	0.96
1:A:245:ASP:HB3	1:A:246:ASN:HB2	1.46	0.94
1:A:245:ASP:CB	1:A:246:ASN:HB3	1.98	0.91
1:A:126:SER:HB3	2:A:1403:SO4:O1	1.69	0.90
1:A:245:ASP:CB	1:A:246:ASN:CB	2.51	0.89
1:B:165:ASN:HD21	1:B:192:ARG:HH11	1.19	0.88
1:A:245:ASP:HB3	1:A:246:ASN:CB	2.02	0.88
1:A:122:ARG:NH2	4:A:1449:HOH:O	2.12	0.81
1:B:52:PHE:CZ	1:B:81:ARG:HD2	2.17	0.80
1:B:128:ASP:N	2:B:2403:SO4:O1	2.20	0.73
1:B:232:LYS:HG2	4:B:2411:HOH:O	1.89	0.72
1:B:165:ASN:ND2	1:B:192:ARG:HH11	1.89	0.71
1:B:246:ASN:HD22	1:B:246:ASN:C	1.92	0.71
1:B:167:VAL:O	1:B:173:ASN:ND2	2.25	0.70
1:B:165:ASN:HD21	1:B:192:ARG:NH1	1.92	0.67
1:A:165:ASN:HD21	1:A:192:ARG:HH11	1.45	0.65
1:B:168:ILE:HA	1:B:173:ASN:HD22	1.63	0.64
1:A:153:ASP:OD2	1:A:187:LYS:NZ	2.32	0.63
1:A:53:ASP:OD1	1:A:89:LYS:HE3	1.98	0.62
1:B:32:MET:HE2	4:B:2415:HOH:O	1.99	0.62
1:B:212:THR:OG1	1:B:215:GLU:HG2	2.01	0.61
1:B:327:ASN:O	1:B:329:GLN:HA	2.00	0.61
1:A:98:ASP:OD1	1:A:122:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HA	1:B:93:ILE:HD12	1.85	0.59
1:B:111:HIS:O	1:B:115:LEU:HG	2.03	0.58
1:A:205:TRP:CD2	1:A:256:VAL:HG22	2.39	0.57
1:B:127:LEU:N	2:B:2403:SO4:O4	2.39	0.56
1:B:178:ILE:HD12	1:B:178:ILE:H	1.71	0.56
1:B:301:LEU:HD22	1:B:305:PHE:CE1	2.43	0.54
1:A:14:ARG:HH21	1:A:69:LYS:NZ	2.06	0.54
1:A:301:LEU:HD22	1:A:305:PHE:CZ	2.43	0.54
1:A:165:ASN:ND2	1:A:192:ARG:HD3	2.23	0.54
1:B:327:ASN:C	1:B:329:GLN:HA	2.28	0.54
1:B:69:LYS:HG2	1:B:98:ASP:HB2	1.90	0.54
1:B:246:ASN:ND2	1:B:246:ASN:C	2.60	0.53
1:A:301:LEU:HD22	1:A:305:PHE:CE1	2.44	0.53
1:A:245:ASP:HB2	1:A:246:ASN:CB	2.23	0.53
1:B:13:ILE:HG12	1:B:309:TRP:CE2	2.43	0.53
1:B:4:GLN:N	4:B:2416:HOH:O	2.42	0.53
1:B:280:PHE:O	1:B:281:ALA:HB2	2.09	0.52
1:A:209:LYS:HD3	1:A:209:LYS:O	2.10	0.52
1:B:259:SER:CB	1:B:318:ASP:OD1	2.58	0.52
1:B:245:ASP:O	1:B:247:GLY:N	2.43	0.51
1:B:279:LEU:HD22	1:B:280:PHE:CE1	2.45	0.51
1:B:166:VAL:HG21	1:B:191:ILE:HD11	1.93	0.51
1:A:71:ARG:HD3	1:A:102:THR:CG2	2.41	0.51
1:A:237:VAL:HG23	1:A:238:ALA:N	2.26	0.51
1:B:205:TRP:CD2	1:B:256:VAL:HG22	2.47	0.50
1:A:278:CYS:HB2	1:A:314:ASP:HB3	1.93	0.50
1:A:47:ASN:H	1:A:47:ASN:ND2	2.10	0.50
1:B:259:SER:HB3	1:B:318:ASP:OD1	2.11	0.50
1:B:237:VAL:HG23	1:B:238:ALA:H	1.77	0.50
1:A:209:LYS:CD	1:A:209:LYS:O	2.60	0.49
1:A:71:ARG:NH1	1:A:102:THR:HG22	2.27	0.49
1:A:202:ASP:N	1:A:203:ASN:HA	2.27	0.49
1:B:28:CYS:HA	1:B:138:ILE:O	2.13	0.48
1:B:136:GLN:HE21	1:B:142:ASN:C	2.17	0.48
1:A:71:ARG:HH11	1:A:102:THR:HG22	1.77	0.48
1:B:219:MET:CE	1:B:219:MET:CG	2.90	0.48
1:B:132:ASP:O	1:B:136:GLN:HG3	2.13	0.47
1:A:116:TYR:C	1:A:116:TYR:CD2	2.88	0.47
1:B:111:HIS:CE1	1:B:114:LYS:HZ3	2.32	0.47
1:B:224:PHE:HB3	1:B:226:ILE:HD13	1.96	0.47
1:B:246:ASN:HD21	1:B:248:VAL:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:CYS:HB2	1:B:318:ASP:OD2	2.15	0.47
1:A:109:LYS:HA	1:A:154:TYR:CE2	2.50	0.46
1:B:5:ILE:HD13	1:B:65:LEU:HD22	1.98	0.46
1:B:320:ARG:O	1:B:324:THR:HG22	2.16	0.46
1:B:168:ILE:O	1:B:196:PHE:HB2	2.16	0.46
1:B:141:ARG:O	1:B:143:ILE:HD13	2.16	0.46
1:A:90:LEU:HA	1:A:93:ILE:HD12	1.98	0.46
1:B:71:ARG:HH11	1:B:102:THR:HG21	1.81	0.46
1:A:213:LYS:NZ	1:B:239:LYS:NZ	2.64	0.46
1:B:147:THR:O	1:B:151:GLN:HG2	2.16	0.45
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.87	0.45
1:A:266:ARG:NH1	1:A:266:ARG:HB2	2.33	0.44
1:B:205:TRP:CD1	1:B:324:THR:HG21	2.52	0.44
1:B:17:ARG:HD2	4:B:2406:HOH:O	2.16	0.44
1:A:278:CYS:HB2	1:A:314:ASP:CB	2.48	0.44
1:A:259:SER:HB3	1:A:318:ASP:OD1	2.19	0.43
1:A:40:ASP:HB2	4:A:1431:HOH:O	2.18	0.43
1:B:245:ASP:OD1	1:B:245:ASP:N	2.52	0.43
1:B:32:MET:HA	1:B:37:PHE:CD1	2.54	0.42
1:B:215:GLU:H	1:B:215:GLU:HG2	1.74	0.42
1:A:301:LEU:CD2	1:A:305:PHE:CZ	3.03	0.42
1:A:328:ARG:NH2	1:B:234:PHE:HB3	2.35	0.41
1:A:218:THR:O	1:A:222:GLN:HG3	2.20	0.41
1:B:27:ARG:O	1:B:140:ASN:HB2	2.20	0.41
1:A:12:PRO:HG3	1:B:326:ALA:HA	2.02	0.41
1:B:196:PHE:CE2	1:B:198:ASP:HB2	2.56	0.41
1:A:261:CYS:HB2	1:A:318:ASP:OD2	2.21	0.41
1:B:178:ILE:HB	1:B:179:PRO:HD3	2.03	0.41
1:A:266:ARG:HH11	1:A:266:ARG:CB	2.33	0.41
1:A:297:THR:OG1	1:A:298:ASP:N	2.53	0.41
1:B:141:ARG:O	1:B:143:ILE:CD1	2.69	0.41
1:B:155:ALA:O	1:B:160:LEU:HB2	2.20	0.41
1:B:238:ALA:HB3	1:B:240:TYR:CE1	2.56	0.40
1:B:130:ILE:HB	1:B:180:MET:HG2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/340 (96%)	307 (94%)	14 (4%)	4 (1%)	16	47
1	B	324/340 (95%)	295 (91%)	22 (7%)	7 (2%)	8	28
All	All	649/680 (95%)	602 (93%)	36 (6%)	11 (2%)	11	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	B	36	VAL
1	B	81	ARG
1	B	246	ASN
1	B	281	ALA
1	B	174	ASP
1	B	245	ASP
1	A	210	VAL
1	A	245	ASP
1	B	315	ARG
1	A	281	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	291/302 (96%)	254 (87%)	37 (13%)	5	16
1	B	290/302 (96%)	255 (88%)	35 (12%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	581/604 (96%)	509 (88%)	72 (12%)	6 17

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	14	ARG
1	A	17	ARG
1	A	18	LEU
1	A	20	VAL
1	A	46	LYS
1	A	81	ARG
1	A	91	ASN
1	A	102	THR
1	A	110	LYS
1	A	120	LEU
1	A	127	LEU
1	A	134	LEU
1	A	149	LEU
1	A	156	THR
1	A	157	SER
1	A	168	ILE
1	A	192	ARG
1	A	202	ASP
1	A	203	ASN
1	A	209	LYS
1	A	210	VAL
1	A	225	GLU
1	A	226	ILE
1	A	242	ARG
1	A	245	ASP
1	A	256	VAL
1	A	258	GLN
1	A	260	PHE
1	A	269	LEU
1	A	282	THR
1	A	292	ILE
1	A	297	THR
1	A	299	GLU
1	A	301	LEU
1	A	311	ILE
1	A	315	ARG

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Mol	Chain	Res	Type
1	B	13	ILE
1	B	20	VAL
1	B	21	THR
1	B	30	TYR
1	B	35	GLU
1	B	42	VAL
1	B	71	ARG
1	B	81	ARG
1	B	83	LEU
1	B	114	LYS
1	B	120	LEU
1	B	134	LEU
1	B	137	SER
1	B	144	LYS
1	B	149	LEU
1	B	168	ILE
1	B	192	ARG
1	B	209	LYS
1	B	215	GLU
1	B	232	LYS
1	B	242	ARG
1	B	246	ASN
1	B	260	PHE
1	B	271	SER
1	B	282	THR
1	B	283	VAL
1	B	299	GLU
1	B	300	GLU
1	B	301	LEU
1	B	303	GLU
1	B	315	ARG
1	B	320	ARG
1	B	324	THR
1	B	328	ARG
1	B	329	GLN

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	4	GLN
1	A	47	ASN
1	A	91	ASN

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Mol	Chain	Res	Type
1	A	165	ASN
1	A	203	ASN
1	B	136	GLN
1	B	165	ASN
1	B	173	ASN
1	B	222	GLN
1	B	246	ASN
1	B	323	GLN
1	B	329	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
3	SF4	A	1401	1,4	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	A	1402	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SO4	A	1403	-	4,4,4	1.96	2 (50%)	6,6,6	0.37	0
3	SF4	B	2401	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	2402	1	0,12,12	0.00	-	0,24,24	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	2403	-	4,4,4	1.89	2 (50%)	6,6,6	0.76	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	SF4	A	1401	1,4	-	0/0/48/48	0/6/5/5
3	SF4	A	1402	1	-	0/0/48/48	0/6/5/5
2	SO4	A	1403	-	-	0/0/0/0	0/0/0/0
3	SF4	B	2401	1	-	0/0/48/48	0/6/5/5
3	SF4	B	2402	1	-	0/0/48/48	0/6/5/5
2	SO4	B	2403	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2403	SO4	O1-S	2.01	1.54	1.47
2	B	2403	SO4	O2-S	2.23	1.54	1.47
2	A	1403	SO4	O3-S	2.25	1.55	1.47
2	A	1403	SO4	O4-S	2.43	1.56	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1403	SO4	1	0
2	B	2403	SO4	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	327/340 (96%)	0.07	6 (1%) 71 61	27, 37, 54, 60	0
1	B	326/340 (95%)	0.33	18 (5%) 29 18	27, 38, 53, 61	0
All	All	653/680 (96%)	0.20	24 (3%) 45 33	27, 37, 54, 61	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	THR	6.2
1	B	41	PHE	4.5
1	B	35	GLU	4.0
1	B	36	VAL	3.7
1	A	246	ASN	3.3
1	A	226	ILE	3.0
1	B	305	PHE	3.0
1	B	283	VAL	2.9
1	A	223	HIS	2.9
1	A	224	PHE	2.8
1	B	301	LEU	2.8
1	B	288	VAL	2.7
1	B	37	PHE	2.7
1	B	286	PHE	2.6
1	B	226	ILE	2.6
1	B	42	VAL	2.6
1	B	44	LEU	2.4
1	A	225	GLU	2.4
1	B	244	LYS	2.3
1	B	296	VAL	2.3
1	B	279	LEU	2.2
1	B	51	THR	2.2
1	A	243	HIS	2.1
1	B	246	ASN	2.1

## 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 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(Å <sup>2</sup> )	Q<0.9
2	SO4	A	1403	5/5	0.98	0.43	6.75	76,80,83,85	0
2	SO4	B	2403	5/5	0.82	0.46	4.13	85,85,91,95	0
3	SF4	B	2402	8/8	0.97	0.10	-1.47	30,34,37,40	0
3	SF4	A	1401	8/8	0.99	0.12	-1.76	34,38,39,39	0
3	SF4	A	1402	8/8	0.99	0.11	-1.99	32,34,35,38	0
3	SF4	B	2401	8/8	0.97	0.05	-2.16	40,45,47,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.