



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:45 AM EDT

PDB ID : 1X9E  
Title : Crystal structure of HMG-CoA synthase from *Enterococcus faecalis*  
Authors : Steussy, C.N.; Vartia, A.A.; Burgner II, J.W.; Sutherlin, A.; Rodwell, V.W.; Stauffacher, C.V.  
Deposited on : 2004-08-20  
Resolution : 2.40 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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

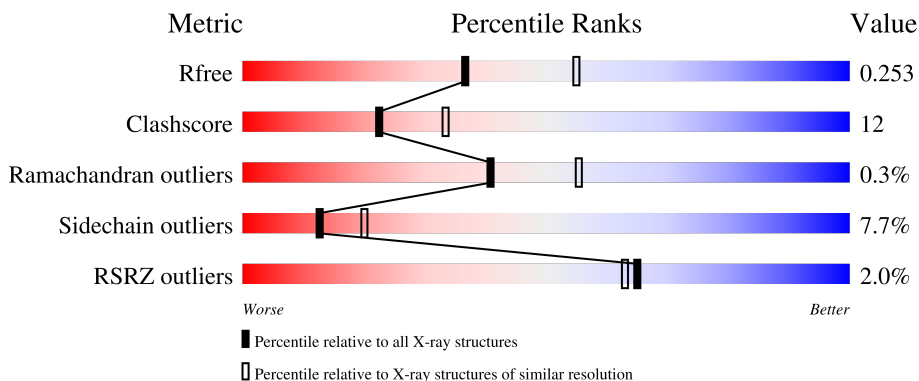
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

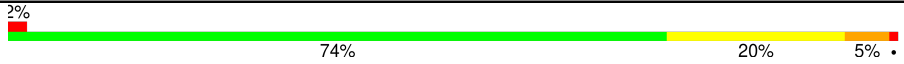
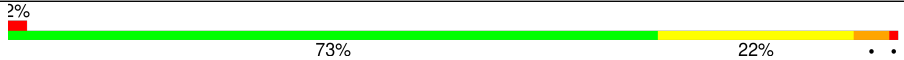
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	383	
1	B	383	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6128 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 HMG-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2969	1886	491	581	11			
1	B	383	Total	C	N	O	S	0	0	0
			2969	1886	491	581	11			

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



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

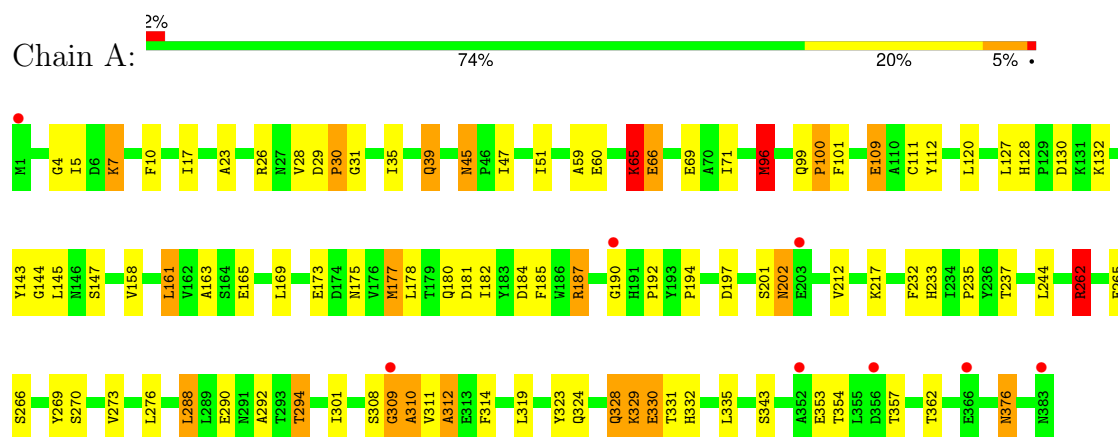
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	87	Total 87	O 87	0	0

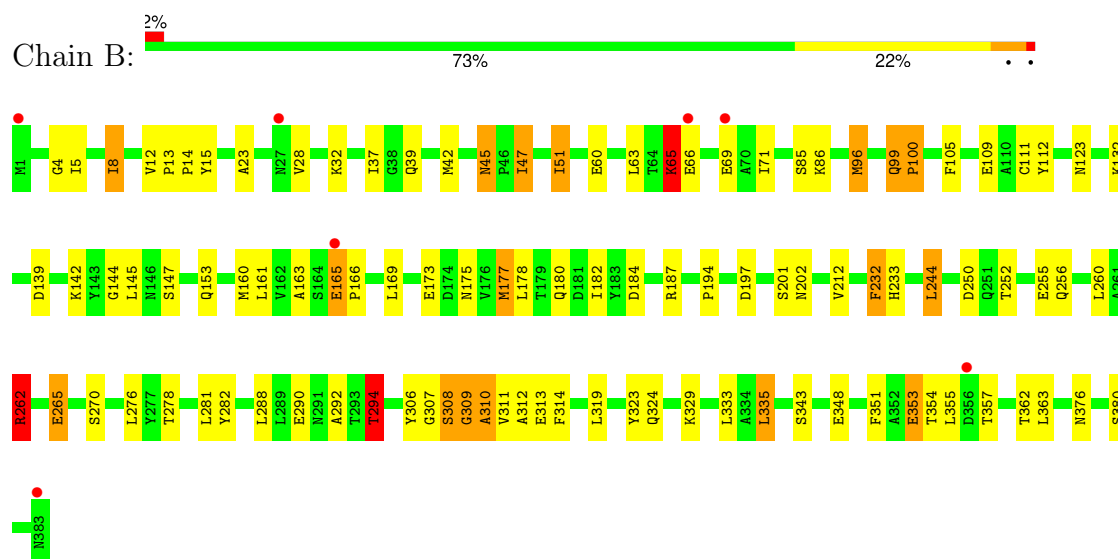
### 3 Residue-property plots

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: HMG-CoA synthase



#### • Molecule 1: HMG-CoA synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.37Å 109.82Å 141.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.50 – 2.40 25.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (26.50-2.40) 97.3 (25.90-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	352.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.225 , 0.254 0.232 , 0.253	Depositor DCC
$R_{free}$ test set	1607 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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

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	1.40	28/3026 (0.9%)	1.24	30/4104 (0.7%)
1	B	1.50	35/3026 (1.2%)	1.29	29/4104 (0.7%)
All	All	1.45	63/6052 (1.0%)	1.27	59/8208 (0.7%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	GLU	CG-CD	-24.68	1.15	1.51
1	B	309	GLY	N-CA	24.27	1.82	1.46
1	A	69	GLU	CG-CD	-24.11	1.15	1.51
1	A	69	GLU	CD-OE1	-17.42	1.06	1.25
1	B	69	GLU	CD-OE1	-16.72	1.07	1.25
1	B	265	GLU	CD-OE2	-16.20	1.07	1.25
1	A	265	GLU	CD-OE2	-15.69	1.08	1.25
1	A	173	GLU	CB-CG	-15.56	1.22	1.52
1	A	202	ASN	CG-OD1	-14.65	0.91	1.24
1	B	173	GLU	CB-CG	-14.41	1.24	1.52
1	B	65	LYS	CD-CE	-14.40	1.15	1.51
1	A	45	ASN	CG-OD1	-14.36	0.92	1.24
1	B	45	ASN	CG-OD1	-14.25	0.92	1.24
1	B	202	ASN	CG-OD1	-13.93	0.93	1.24
1	A	173	GLU	CD-OE2	-13.76	1.10	1.25
1	A	65	LYS	CD-CE	-13.69	1.17	1.51
1	A	45	ASN	CG-ND2	-13.43	0.99	1.32
1	B	45	ASN	CG-ND2	-13.15	0.99	1.32
1	B	173	GLU	CG-CD	-13.00	1.32	1.51
1	B	173	GLU	CD-OE2	-12.56	1.11	1.25
1	B	276	LEU	CG-CD1	-12.35	1.06	1.51
1	A	276	LEU	CG-CD1	-12.27	1.06	1.51
1	A	276	LEU	CG-CD2	-12.09	1.07	1.51
1	A	51	ILE	CB-CG2	-12.04	1.15	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	ILE	CB-CG2	-12.04	1.15	1.52
1	A	173	GLU	CG-CD	-11.86	1.34	1.51
1	B	309	GLY	C-O	-11.83	1.04	1.23
1	B	276	LEU	CG-CD2	-11.24	1.10	1.51
1	B	265	GLU	CD-OE1	-11.02	1.13	1.25
1	B	262	ARG	NE-CZ	-10.36	1.19	1.33
1	A	265	GLU	CD-OE1	-10.34	1.14	1.25
1	A	165	GLU	CD-OE1	-10.16	1.14	1.25
1	A	66	GLU	CD-OE2	-10.05	1.14	1.25
1	B	66	GLU	CD-OE2	-9.80	1.14	1.25
1	B	165	GLU	CD-OE1	-8.86	1.15	1.25
1	B	66	GLU	CD-OE1	-8.74	1.16	1.25
1	A	262	ARG	NE-CZ	-8.73	1.21	1.33
1	B	202	ASN	CG-ND2	-8.23	1.12	1.32
1	A	51	ILE	CB-CG1	-8.13	1.31	1.54
1	A	202	ASN	CG-ND2	-8.12	1.12	1.32
1	B	51	ILE	CB-CG1	-8.00	1.31	1.54
1	A	173	GLU	CD-OE1	-7.97	1.16	1.25
1	B	311	VAL	C-N	7.75	1.51	1.34
1	A	99	GLN	CD-OE1	-7.74	1.06	1.24
1	A	66	GLU	CD-OE1	-7.65	1.17	1.25
1	B	99	GLN	CD-OE1	-7.58	1.07	1.24
1	A	96	MET	SD-CE	-7.53	1.35	1.77
1	B	262	ARG	CZ-NH1	-7.05	1.23	1.33
1	A	99	GLN	CD-NE2	-6.41	1.16	1.32
1	B	262	ARG	CZ-NH2	-6.39	1.24	1.33
1	A	294	THR	CB-CG2	-6.37	1.31	1.52
1	B	173	GLU	CD-OE1	-6.30	1.18	1.25
1	B	308	SER	CA-C	-6.29	1.36	1.52
1	B	308	SER	C-N	6.27	1.44	1.33
1	B	99	GLN	CD-NE2	-6.09	1.17	1.32
1	B	96	MET	SD-CE	-5.84	1.45	1.77
1	A	262	ARG	CZ-NH2	-5.65	1.25	1.33
1	A	165	GLU	CD-OE2	-5.63	1.19	1.25
1	B	306	TYR	C-N	5.58	1.43	1.33
1	B	294	THR	CB-CG2	-5.33	1.34	1.52
1	B	262	ARG	CD-NE	-5.18	1.37	1.46
1	B	51	ILE	CG1-CD1	-5.12	1.15	1.50
1	A	312	ALA	C-N	5.11	1.45	1.34

All (59) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ARG	NE-CZ-NH1	-17.70	111.45	120.30
1	A	262	ARG	NE-CZ-NH1	-15.43	112.58	120.30
1	A	265	GLU	OE1-CD-OE2	-13.10	107.58	123.30
1	B	262	ARG	NH1-CZ-NH2	12.70	133.37	119.40
1	A	262	ARG	NH1-CZ-NH2	12.47	133.12	119.40
1	B	265	GLU	OE1-CD-OE2	-12.47	108.34	123.30
1	A	262	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	B	69	GLU	CG-CD-OE1	-12.01	94.27	118.30
1	B	69	GLU	OE1-CD-OE2	11.99	137.69	123.30
1	A	69	GLU	CG-CD-OE1	-11.87	94.55	118.30
1	A	69	GLU	OE1-CD-OE2	11.53	137.14	123.30
1	B	262	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	51	ILE	CG1-CB-CG2	-10.01	89.39	111.40
1	B	307	GLY	O-C-N	9.64	138.13	122.70
1	A	66	GLU	OE1-CD-OE2	-9.30	112.14	123.30
1	A	51	ILE	CG1-CB-CG2	-9.29	90.97	111.40
1	B	309	GLY	CA-C-O	-8.46	105.37	120.60
1	B	66	GLU	OE1-CD-OE2	-8.25	113.40	123.30
1	B	312	ALA	O-C-N	8.06	135.60	122.70
1	B	310	ALA	N-CA-CB	7.84	121.08	110.10
1	A	309	GLY	N-CA-C	7.52	131.89	113.10
1	B	311	VAL	O-C-N	7.17	134.17	122.70
1	A	310	ALA	N-CA-CB	7.17	120.13	110.10
1	B	276	LEU	CD1-CG-CD2	-7.10	89.20	110.50
1	A	276	LEU	CD1-CG-CD2	-6.95	89.64	110.50
1	B	233	HIS	N-CA-C	-6.85	92.51	111.00
1	A	51	ILE	CB-CG1-CD1	-6.75	94.99	113.90
1	B	100	PRO	N-CA-C	6.66	129.42	112.10
1	A	262	ARG	CD-NE-CZ	-6.65	114.29	123.60
1	A	233	HIS	N-CA-C	-6.64	93.06	111.00
1	B	311	VAL	C-N-CA	-6.50	105.45	121.70
1	B	276	LEU	CB-CG-CD1	6.45	121.97	111.00
1	A	235	PRO	N-CA-C	-6.41	95.42	112.10
1	A	100	PRO	N-CA-C	6.41	128.75	112.10
1	A	265	GLU	CG-CD-OE1	6.37	131.05	118.30
1	B	197	ASP	N-CA-C	-6.34	93.87	111.00
1	A	197	ASP	N-CA-C	-6.24	94.17	111.00
1	B	265	GLU	CG-CD-OE1	6.18	130.65	118.30
1	A	276	LEU	CB-CG-CD2	6.05	121.28	111.00
1	A	165	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	A	276	LEU	CB-CG-CD1	5.96	121.13	111.00
1	B	312	ALA	C-N-CA	-5.84	107.09	121.70
1	B	65	LYS	CD-CE-NZ	5.83	125.12	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	B	175	ASN	N-CA-C	5.55	125.98	111.00
1	A	65	LYS	CD-CE-NZ	5.55	124.46	111.70
1	B	312	ALA	N-CA-C	-5.45	96.28	111.00
1	A	232	PHE	CB-CA-C	-5.41	99.57	110.40
1	A	237	THR	N-CA-C	5.37	125.49	111.00
1	B	307	GLY	C-N-CA	-5.25	108.57	121.70
1	A	173	GLU	CA-CB-CG	5.24	124.92	113.40
1	A	175	ASN	N-CA-C	5.23	125.11	111.00
1	B	343	SER	N-CA-C	-5.20	96.96	111.00
1	A	161	LEU	N-CA-C	-5.18	97.01	111.00
1	B	85	SER	N-CA-CB	-5.11	102.83	110.50
1	B	232	PHE	CB-CA-C	-5.08	100.25	110.40
1	A	343	SER	N-CA-C	-5.05	97.37	111.00
1	A	312	ALA	N-CA-CB	5.04	117.16	110.10
1	A	69	GLU	CG-CD-OE2	5.00	128.31	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	2969	0	2929	74	0
1	B	2969	0	2929	67	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	A	83	0	0	8	0
3	B	87	0	0	2	0
All	All	6128	0	5858	137	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 12.

All (137) 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:309:GLY:N	1:B:309:GLY:CA	1.82	1.38
1:B:262:ARG:HH22	1:B:294:THR:HB	1.20	1.02
1:A:290:GLU:HB3	1:A:329:LYS:HG3	1.60	0.82
1:B:47:ILE:HD11	1:B:353:GLU:CD	2.03	0.79
1:B:250:ASP:OD1	3:B:419:HOH:O	2.04	0.76
1:A:329:LYS:O	1:A:332:HIS:HB2	1.86	0.75
1:A:65:LYS:HE3	1:A:65:LYS:CA	2.17	0.74
1:A:65:LYS:HE3	1:A:65:LYS:N	2.04	0.72
1:A:29:ASP:O	1:A:31:GLY:N	2.22	0.72
1:B:42:MET:HE1	1:B:153:GLN:HE21	1.54	0.72
1:B:60:GLU:HA	1:B:96:MET:HE1	1.72	0.71
1:B:42:MET:CE	1:B:153:GLN:HE21	2.04	0.70
1:B:308:SER:HB2	3:B:405:HOH:O	1.92	0.70
1:B:8:ILE:HG22	1:B:160:MET:HG2	1.73	0.69
1:A:30:PRO:O	3:A:456:HOH:O	2.12	0.68
1:A:309:GLY:N	1:A:310:ALA:HA	2.10	0.65
1:B:309:GLY:N	1:B:310:ALA:HA	2.12	0.64
1:A:212:VAL:CG1	1:A:314:PHE:HB2	2.28	0.64
1:A:26:ARG:O	1:A:28:VAL:HG13	1.98	0.62
1:B:5:ILE:CG2	1:B:8:ILE:HG23	2.29	0.62
1:A:29:ASP:O	1:A:30:PRO:C	2.40	0.60
1:A:35:ILE:O	1:A:35:ILE:HG22	2.00	0.60
1:B:145:LEU:HD23	1:B:348:GLU:HG2	1.82	0.60
1:B:65:LYS:H	1:B:65:LYS:HE2	1.67	0.60
1:B:252:THR:OG1	1:B:255:GLU:HB2	2.02	0.60
1:A:128:HIS:HE1	3:A:468:HOH:O	1.85	0.60
1:B:63:LEU:HD12	1:B:96:MET:HE3	1.84	0.59
1:A:290:GLU:OE1	1:A:329:LYS:HA	2.03	0.59
1:A:180:GLN:O	1:A:310:ALA:N	2.33	0.59
1:A:319:LEU:HD12	1:A:323:TYR:CE1	2.39	0.58
1:A:185:PHE:HB3	1:A:308:SER:HB3	1.85	0.58
1:B:42:MET:HE3	1:B:153:GLN:HB2	1.84	0.58
1:A:59:ALA:HB3	1:A:96:MET:HE2	1.85	0.58
1:A:329:LYS:O	1:A:332:HIS:N	2.37	0.57
1:B:308:SER:C	1:B:309:GLY:CA	2.71	0.57
1:B:362:THR:HG22	1:B:363:LEU:N	2.20	0.57
1:B:42:MET:HE1	1:B:153:GLN:NE2	2.19	0.57
1:A:143:TYR:HE2	3:A:467:HOH:O	1.86	0.56
1:A:65:LYS:N	1:A:65:LYS:CE	2.68	0.56
1:B:112:TYR:OH	1:B:313:GLU:OE1	2.21	0.56
1:A:187:ARG:HG3	1:A:194:PRO:HA	1.89	0.55
1:A:66:GLU:OE1	1:A:66:GLU:N	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:HB2	1:B:201:SER:HA	1.87	0.55
1:A:39:GLN:HG3	3:A:400:HOH:O	2.05	0.55
1:B:65:LYS:H	1:B:65:LYS:CE	2.20	0.54
1:B:232:PHE:CE1	1:B:244:LEU:CD2	2.91	0.54
1:B:262:ARG:HH22	1:B:294:THR:CB	2.08	0.54
1:B:319:LEU:HD13	1:B:323:TYR:CZ	2.43	0.54
1:A:328:GLN:HE21	1:A:328:GLN:HA	1.73	0.54
1:B:8:ILE:CG2	1:B:160:MET:HG2	2.37	0.53
1:A:319:LEU:HD12	1:A:323:TYR:CD1	2.44	0.53
1:B:182:ILE:O	1:B:309:GLY:HA2	2.08	0.53
1:B:290:GLU:O	1:B:329:LYS:HE3	2.08	0.53
1:A:59:ALA:CB	1:A:96:MET:HE2	2.39	0.53
1:B:232:PHE:CZ	1:B:244:LEU:HD22	2.44	0.53
1:B:71:ILE:HA	1:B:132:LYS:O	2.10	0.52
1:A:181:ASP:OD1	1:B:86:LYS:NZ	2.39	0.52
1:A:185:PHE:HB3	1:A:308:SER:CB	2.39	0.52
1:B:63:LEU:HD12	1:B:96:MET:CE	2.39	0.52
1:A:59:ALA:HB3	1:A:96:MET:CE	2.39	0.52
1:A:328:GLN:O	1:A:329:LYS:C	2.48	0.52
1:B:4:GLY:HA3	1:B:169:LEU:O	2.09	0.52
1:B:5:ILE:HG21	1:B:8:ILE:CG2	2.41	0.51
1:A:65:LYS:HE3	1:A:65:LYS:HA	1.93	0.51
1:A:184:ASP:OD1	1:A:309:GLY:N	2.43	0.51
1:A:266:SER:HB3	1:A:288:LEU:HD13	1.92	0.50
1:A:288:LEU:O	1:A:292:ALA:HB3	2.11	0.50
1:A:145:LEU:HD12	3:A:406:HOH:O	2.12	0.50
1:A:328:GLN:HB2	1:A:332:HIS:CE1	2.46	0.50
1:B:362:THR:HG22	1:B:363:LEU:H	1.75	0.49
1:A:35:ILE:O	1:A:35:ILE:CG2	2.60	0.49
1:A:331:THR:O	1:A:335:LEU:HB2	2.13	0.49
1:B:262:ARG:NH2	1:B:294:THR:HB	2.05	0.48
1:A:301:ILE:HD11	1:A:319:LEU:HD21	1.94	0.48
1:B:281:LEU:HD23	1:B:282:TYR:CE2	2.48	0.48
1:B:145:LEU:CD2	1:B:348:GLU:HG2	2.44	0.48
1:B:28:VAL:HG23	1:B:32:LYS:HD2	1.95	0.48
1:A:182:ILE:O	1:A:309:GLY:HA2	2.13	0.48
1:A:127:LEU:HD12	1:B:123:ASN:OD1	2.14	0.48
1:A:177:MET:HE3	3:A:452:HOH:O	2.13	0.48
1:A:120:LEU:HD11	1:B:105:PHE:CZ	2.49	0.47
1:A:47:ILE:HD11	1:A:353:GLU:CD	2.35	0.47
1:A:308:SER:C	1:A:310:ALA:HA	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TYR:O	1:A:273:VAL:HG23	2.15	0.47
1:B:180:GLN:O	1:B:310:ALA:N	2.47	0.47
1:B:5:ILE:HG21	1:B:8:ILE:HG23	1.96	0.46
1:B:308:SER:C	1:B:310:ALA:HA	2.36	0.46
1:B:60:GLU:CA	1:B:96:MET:HE1	2.42	0.46
1:B:232:PHE:CZ	1:B:244:LEU:CD2	2.98	0.46
1:B:5:ILE:CG2	1:B:8:ILE:CG2	2.93	0.46
1:B:256:GLN:O	1:B:260:LEU:HG	2.15	0.46
1:B:212:VAL:CG1	1:B:314:PHE:HB2	2.46	0.46
1:B:28:VAL:CG2	1:B:32:LYS:HD2	2.45	0.46
1:B:132:LYS:HG2	1:B:163:ALA:HB2	1.97	0.46
1:B:42:MET:HE3	1:B:153:GLN:CB	2.46	0.46
1:A:71:ILE:HA	1:A:132:LYS:O	2.16	0.45
1:B:12:VAL:HG22	1:B:335:LEU:HD23	1.97	0.45
1:A:217:LYS:NZ	3:A:464:HOH:O	2.49	0.45
1:A:184:ASP:HB2	1:A:201:SER:HA	1.97	0.45
1:A:144:GLY:O	1:A:147:SER:OG	2.35	0.45
1:A:262:ARG:HA	1:A:262:ARG:HD3	1.85	0.45
1:A:112:TYR:CD2	1:A:311:VAL:HG11	2.52	0.44
1:A:4:GLY:HA3	1:A:169:LEU:O	2.17	0.44
1:A:311:VAL:HG12	1:A:312:ALA:N	2.31	0.44
1:A:130:ASP:OD1	1:A:130:ASP:N	2.46	0.44
1:B:354:THR:HG22	1:B:355:LEU:N	2.33	0.44
1:B:142:LYS:HD3	1:B:351:PHE:CE2	2.53	0.44
1:B:187:ARG:HG3	1:B:194:PRO:HA	2.00	0.44
1:A:132:LYS:HG2	1:A:163:ALA:HB2	2.00	0.43
1:B:13:PRO:HG3	1:B:45:ASN:HB3	2.00	0.43
1:B:65:LYS:HE2	1:B:65:LYS:HB2	1.91	0.43
1:A:5:ILE:HD12	1:A:169:LEU:HD23	2.01	0.43
1:B:265:GLU:OE2	1:B:292:ALA:HA	2.19	0.42
1:A:177:MET:CE	3:A:452:HOH:O	2.67	0.42
1:A:7:LYS:NZ	2:A:384:SO4:O1	2.48	0.42
1:B:144:GLY:O	1:B:147:SER:OG	2.38	0.42
1:A:23:ALA:CB	1:A:30:PRO:HA	2.50	0.42
1:A:330:GLU:H	1:A:330:GLU:HG3	1.22	0.42
1:B:51:ILE:HA	1:B:51:ILE:HD13	1.79	0.42
1:A:29:ASP:C	1:A:31:GLY:N	2.72	0.42
1:B:14:PRO:HG2	1:B:15:TYR:CE2	2.55	0.42
1:A:60:GLU:N	1:A:96:MET:CE	2.83	0.41
1:A:112:TYR:CE2	1:A:311:VAL:HG11	2.55	0.41
1:A:262:ARG:HD3	1:A:262:ARG:HH11	1.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:CB	1:A:288:LEU:HD13	2.51	0.41
1:A:328:GLN:HE21	1:A:328:GLN:CA	2.33	0.41
1:A:101:PHE:HA	1:B:177:MET:O	2.21	0.41
1:A:190:GLY:O	1:A:192:PRO:HD3	2.21	0.41
1:B:165:GLU:N	1:B:166:PRO:CD	2.82	0.41
1:A:10:PHE:HB3	1:A:158:VAL:HG22	2.03	0.41
1:B:37:ILE:HD13	1:B:37:ILE:HA	1.91	0.41
1:B:23:ALA:HA	1:B:28:VAL:HG13	2.02	0.41
1:A:17:ILE:O	1:A:17:ILE:HG13	2.21	0.40
1:B:139:ASP:OD2	1:B:278:THR:OG1	2.32	0.40
1:A:109:GLU:HG3	1:A:311:VAL:HG21	2.03	0.40
1:A:329:LYS:O	1:A:332:HIS:CB	2.63	0.40
1:A:376:ASN:HD22	1:A:376:ASN:HA	1.65	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	381/383 (100%)	365 (96%)	14 (4%)	2 (0%)	29	41
1	B	381/383 (100%)	367 (96%)	14 (4%)	0	100	100
All	All	762/766 (100%)	732 (96%)	28 (4%)	2 (0%)	41	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	329	LYS

### 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	312/312 (100%)	287 (92%)	25 (8%)	12	18
1	B	312/312 (100%)	289 (93%)	23 (7%)	13	22
All	All	624/624 (100%)	576 (92%)	48 (8%)	13	20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	39	GLN
1	A	45	ASN
1	A	65	LYS
1	A	96	MET
1	A	100	PRO
1	A	109	GLU
1	A	111	CYS
1	A	161	LEU
1	A	177	MET
1	A	178	LEU
1	A	187	ARG
1	A	202	ASN
1	A	244	LEU
1	A	262	ARG
1	A	270	SER
1	A	288	LEU
1	A	294	THR
1	A	324	GLN
1	A	328	GLN
1	A	330	GLU
1	A	354	THR
1	A	357	THR
1	A	362	THR
1	A	376	ASN
1	B	8	ILE
1	B	39	GLN

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Mol	Chain	Res	Type
1	B	47	ILE
1	B	65	LYS
1	B	99	GLN
1	B	100	PRO
1	B	109	GLU
1	B	111	CYS
1	B	161	LEU
1	B	177	MET
1	B	178	LEU
1	B	244	LEU
1	B	262	ARG
1	B	270	SER
1	B	288	LEU
1	B	294	THR
1	B	324	GLN
1	B	333	LEU
1	B	335	LEU
1	B	353	GLU
1	B	357	THR
1	B	376	ASN
1	B	380	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	202	ASN
1	A	324	GLN
1	A	328	GLN
1	A	338	ASN
1	A	376	ASN
1	B	153	GLN
1	B	328	GLN
1	B	338	ASN
1	B	376	ASN

### 5.3.3 RNA ⓘ

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](#)

4 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	A	385	-	4,4,4	0.53	0	6,6,6	0.11	0
2	SO4	A	384	-	4,4,4	0.50	0	6,6,6	0.17	0
2	SO4	B	384	-	4,4,4	0.47	0	6,6,6	0.10	0
2	SO4	B	385	-	4,4,4	0.42	0	6,6,6	0.13	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	384	SO4	1	0

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	383/383 (100%)	-0.05	8 (2%) 63 61	9, 18, 29, 38	0
1	B	383/383 (100%)	-0.02	7 (1%) 68 66	9, 19, 29, 38	0
All	All	766/766 (100%)	-0.04	15 (1%) 65 63	9, 18, 29, 38	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	ASN	4.5
1	A	190	GLY	3.8
1	A	1	MET	2.9
1	A	203	GLU	2.8
1	B	1	MET	2.6
1	A	356	ASP	2.6
1	B	66	GLU	2.5
1	A	366	GLU	2.5
1	A	352	ALA	2.4
1	A	309	GLY	2.4
1	B	356	ASP	2.4
1	B	165	GLU	2.3
1	A	383	ASN	2.2
1	B	69	GLU	2.1
1	B	27	ASN	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	A	385	5/5	0.92	0.21	15,15,15,15	5
2	SO4	A	384	5/5	0.95	0.16	45,45,46,47	0
2	SO4	B	384	5/5	0.95	0.13	12,13,13,13	5
2	SO4	B	385	5/5	0.96	0.18	44,45,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.