



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 04:23 PM UTC

PDB ID : 1X9E / pdb_00001x9e
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

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

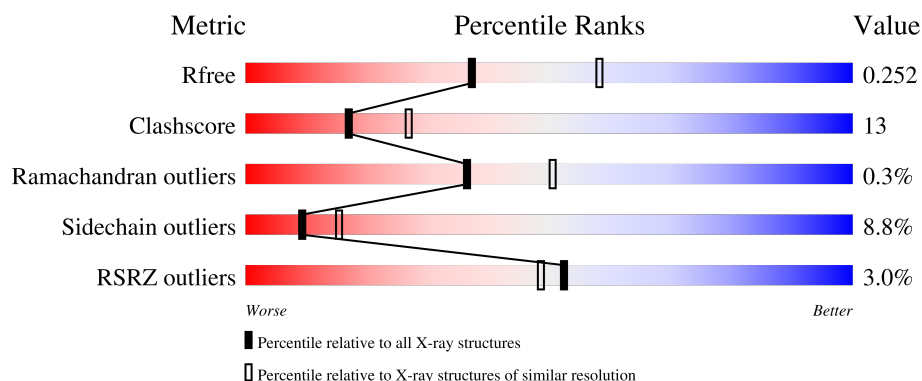
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 ≥ 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	3% 63% 27% 8% .
1	B	383	3% 62% 30% 7% .

2 Entry composition [i](#)

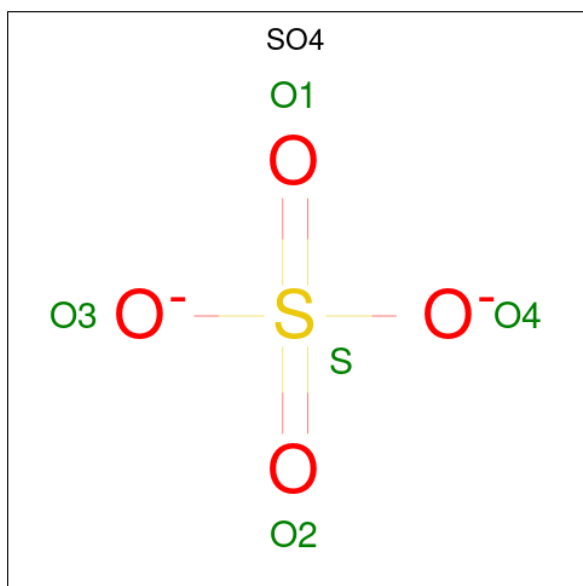
There are 3 unique types of molecules in this entry. The entry contains 6128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



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		

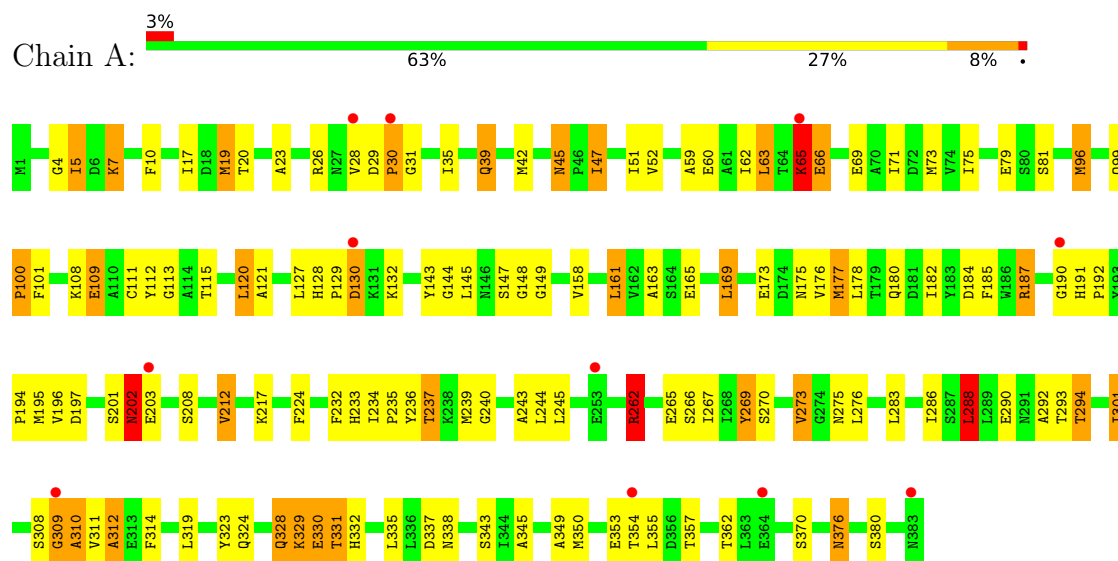
- Molecule 3 is water.

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

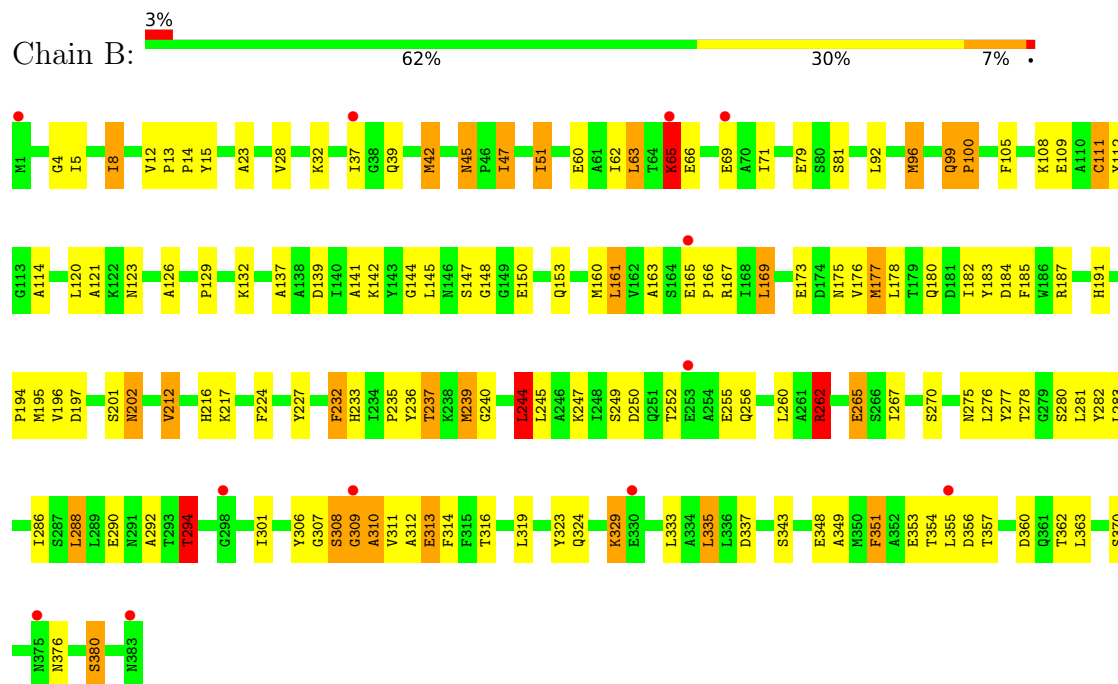
3 Residue-property plots [i](#)

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: 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, α , β , γ	105.37Å 109.82Å 141.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.50 – 2.40 26.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (26.50-2.40) 97.3 (26.50-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	352.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.254 0.232 , 0.252	Depositor DCC
R_{free} test set	1607 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.22$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.48	34/3026 (1.1%)	1.63	80/4104 (1.9%)
1	B	1.63	48/3026 (1.6%)	1.70	94/4104 (2.3%)
All	All	1.56	82/6052 (1.4%)	1.66	174/8208 (2.1%)

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	GLY	N-CA	26.86	1.82	1.45
1	A	96	MET	SD-CE	-17.54	1.35	1.79
1	A	202	ASN	CG-OD1	-16.75	0.91	1.23
1	A	45	ASN	CG-OD1	-16.41	0.92	1.23
1	B	45	ASN	CG-OD1	-16.29	0.92	1.23
1	A	45	ASN	CG-ND2	-16.18	0.99	1.33
1	B	202	ASN	CG-OD1	-15.92	0.93	1.23
1	B	45	ASN	CG-ND2	-15.85	0.99	1.33
1	B	69	GLU	CG-CD	-14.85	1.15	1.52
1	A	69	GLU	CG-CD	-14.51	1.15	1.52
1	B	311	VAL	C-N	14.33	1.51	1.33
1	B	276	LEU	CG-CD1	-14.05	1.06	1.52
1	A	276	LEU	CG-CD1	-13.96	1.06	1.52
1	B	96	MET	SD-CE	-13.77	1.45	1.79
1	A	276	LEU	CG-CD2	-13.76	1.07	1.52
1	B	309	GLY	C-O	-13.31	1.04	1.24
1	B	276	LEU	CG-CD2	-12.82	1.10	1.52
1	B	308	SER	CA-C	-12.75	1.36	1.52
1	B	65	LYS	CD-CE	-12.40	1.15	1.52
1	B	262	ARG	NE-CZ	-12.24	1.19	1.33
1	A	65	LYS	CD-CE	-11.81	1.17	1.52
1	A	51	ILE	CB-CG2	-11.22	1.15	1.52
1	B	51	ILE	CB-CG2	-11.22	1.15	1.52
1	A	51	ILE	CB-CG1	-11.09	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	ILE	CB-CG1	-10.90	1.31	1.53
1	A	262	ARG	NE-CZ	-10.32	1.21	1.33
1	B	202	ASN	CG-ND2	-9.99	1.12	1.33
1	A	173	GLU	CB-CG	-9.95	1.22	1.52
1	A	69	GLU	CD-OE1	-9.93	1.06	1.25
1	A	312	ALA	C-N	9.90	1.45	1.33
1	A	202	ASN	CG-ND2	-9.86	1.12	1.33
1	B	69	GLU	CD-OE1	-9.52	1.07	1.25
1	B	51	ILE	CG1-CD1	-9.40	1.15	1.51
1	B	173	GLU	CB-CG	-9.23	1.24	1.52
1	B	265	GLU	CD-OE2	-9.22	1.07	1.25
1	A	191	HIS	CE1-NE2	-9.17	1.23	1.32
1	A	265	GLU	CD-OE2	-8.93	1.08	1.25
1	A	99	GLN	CD-OE1	-8.74	1.06	1.23
1	B	99	GLN	CD-OE1	-8.56	1.07	1.23
1	B	191	HIS	CE1-NE2	-8.38	1.24	1.32
1	A	51	ILE	CG1-CD1	-8.18	1.19	1.51
1	B	173	GLU	CG-CD	-7.84	1.32	1.52
1	A	99	GLN	CD-NE2	-7.82	1.16	1.33
1	A	173	GLU	CD-OE2	-7.81	1.10	1.25
1	B	42	MET	SD-CE	-7.45	1.60	1.79
1	B	99	GLN	CD-NE2	-7.44	1.17	1.33
1	B	313	GLU	N-CA	7.23	1.54	1.46
1	B	308	SER	C-O	7.18	1.32	1.23
1	A	173	GLU	CG-CD	-7.16	1.34	1.52
1	B	173	GLU	CD-OE2	-7.11	1.11	1.25
1	B	197	ASP	CA-C	6.87	1.61	1.52
1	B	308	SER	C-N	6.81	1.44	1.33
1	B	262	ARG	CZ-NH2	-6.70	1.24	1.33
1	B	310	ALA	C-N	6.59	1.42	1.33
1	B	307	GLY	C-N	6.58	1.42	1.33
1	B	306	TYR	C-N	6.57	1.43	1.33
1	A	294	THR	CB-CG2	-6.43	1.31	1.52
1	B	191	HIS	CG-CD2	-6.38	1.28	1.35
1	B	262	ARG	CZ-NH1	-6.33	1.23	1.32
1	B	283	LEU	CA-C	6.29	1.60	1.52
1	B	265	GLU	CD-OE1	-6.22	1.13	1.25
1	B	311	VAL	C-O	6.16	1.31	1.23
1	B	262	ARG	CD-NE	-6.15	1.37	1.46
1	A	191	HIS	CG-CD2	-6.01	1.29	1.35
1	A	262	ARG	CZ-NH2	-5.96	1.25	1.33
1	A	265	GLU	CD-OE1	-5.83	1.14	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	ARG	CD-NE	-5.82	1.38	1.46
1	A	309	GLY	CA-C	5.75	1.59	1.52
1	A	165	GLU	CD-OE1	-5.72	1.14	1.25
1	B	312	ALA	N-CA	5.71	1.53	1.45
1	A	66	GLU	CD-OE2	-5.66	1.14	1.25
1	B	311	VAL	N-CA	5.55	1.52	1.46
1	B	66	GLU	CD-OE2	-5.51	1.14	1.25
1	A	99	GLN	CA-CB	5.44	1.61	1.53
1	B	294	THR	CB-CG2	-5.39	1.34	1.52
1	A	191	HIS	CG-ND1	-5.34	1.32	1.38
1	B	65	LYS	C-N	-5.33	1.26	1.33
1	B	286	ILE	CA-CB	5.30	1.60	1.54
1	B	310	ALA	N-CA	5.29	1.56	1.46
1	A	286	ILE	CA-CB	5.23	1.60	1.54
1	B	99	GLN	CA-CB	5.14	1.60	1.53
1	A	73	MET	SD-CE	-5.07	1.66	1.79

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	GLY	N-CA-C	15.47	131.89	113.79
1	B	309	GLY	CA-C-O	-13.76	105.37	119.27
1	B	233	HIS	N-CA-C	-12.14	92.51	110.48
1	B	307	GLY	O-C-N	11.87	138.13	122.70
1	A	233	HIS	N-CA-C	-11.77	93.06	110.48
1	A	100	PRO	N-CA-C	10.95	128.75	113.53
1	B	312	ALA	O-C-N	10.87	135.60	123.10
1	B	262	ARG	NH1-CZ-NH2	10.82	133.37	119.30
1	A	262	ARG	NH1-CZ-NH2	10.63	133.12	119.30
1	B	100	PRO	N-CA-C	10.52	129.42	113.75
1	B	69	GLU	CG-CD-OE1	-10.49	94.27	118.40
1	B	311	VAL	O-C-N	10.47	134.17	122.97
1	B	175	ASN	N-CA-C	10.45	125.98	110.30
1	A	79	GLU	N-CA-C	-10.45	98.09	112.30
1	B	235	PRO	N-CA-C	-10.38	99.75	114.18
1	A	69	GLU	CG-CD-OE1	-10.37	94.55	118.40
1	B	196	VAL	N-CA-C	10.34	123.07	107.77
1	B	308	SER	N-CA-C	10.19	124.21	110.35
1	B	262	ARG	NE-CZ-NH1	-10.05	111.45	121.50
1	B	311	VAL	CA-C-N	-10.01	105.45	121.87
1	B	311	VAL	C-N-CA	-10.01	105.45	121.87
1	A	175	ASN	N-CA-C	9.88	125.11	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	LEU	CD1-CG-CD2	-9.82	89.20	110.80
1	A	283	LEU	N-CA-C	-9.70	99.76	111.69
1	A	276	LEU	CD1-CG-CD2	-9.62	89.64	110.80
1	B	283	LEU	N-CA-C	-9.55	100.95	111.36
1	B	311	VAL	CA-C-O	-9.41	110.65	121.75
1	B	343	SER	N-CA-C	-9.40	96.96	110.59
1	A	343	SER	N-CA-C	-9.12	97.37	110.59
1	A	51	ILE	CB-CG1-CD1	-8.96	94.99	113.80
1	A	196	VAL	N-CA-C	8.95	121.00	108.12
1	A	262	ARG	NE-CZ-NH1	-8.91	112.58	121.50
1	A	267	ILE	N-CA-C	8.85	119.79	111.91
1	A	331	THR	N-CA-C	-8.58	101.92	111.28
1	A	237	THR	N-CA-C	8.55	125.49	111.37
1	B	312	ALA	N-CA-C	-8.51	96.28	108.96
1	A	232	PHE	N-CA-C	8.43	122.81	109.50
1	B	79	GLU	N-CA-C	-8.41	99.84	112.54
1	B	197	ASP	N-CA-C	-8.38	93.87	108.20
1	A	63	LEU	N-CA-C	8.34	123.01	109.76
1	A	235	PRO	N-CA-C	-8.28	95.42	112.47
1	B	308	SER	CA-C-N	-8.23	111.97	123.08
1	B	308	SER	C-N-CA	-8.23	111.97	123.08
1	A	148	GLY	N-CA-C	-8.13	102.66	112.49
1	B	307	GLY	CA-C-N	-8.07	108.57	120.75
1	B	307	GLY	C-N-CA	-8.07	108.57	120.75
1	A	20	THR	N-CA-C	-7.97	102.67	111.36
1	B	312	ALA	CA-C-N	-7.89	107.09	121.69
1	B	312	ALA	C-N-CA	-7.89	107.09	121.69
1	B	148	GLY	N-CA-C	-7.81	103.04	112.49
1	B	329	LYS	N-CA-C	7.70	120.65	111.33
1	B	237	THR	N-CA-C	7.26	123.34	111.37
1	A	262	ARG	CD-NE-CZ	-7.22	114.29	124.40
1	A	161	LEU	N-CA-C	-7.19	97.01	108.73
1	A	45	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	B	310	ALA	N-CA-CB	7.12	121.08	110.40
1	A	121	ALA	N-CA-C	-7.12	103.60	111.36
1	B	45	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	B	51	ILE	CG1-CB-CG2	-7.11	89.39	110.70
1	B	224	PHE	N-CA-C	7.09	119.01	111.28
1	B	120	LEU	N-CA-C	-7.07	103.66	111.36
1	B	63	LEU	N-CA-C	7.01	121.10	109.46
1	B	232	PHE	N-CA-C	7.00	120.91	109.72
1	A	245	LEU	N-CA-C	6.94	119.44	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	MET	N-CA-C	-6.88	98.02	109.24
1	B	240	GLY	N-CA-C	-6.87	104.16	113.37
1	A	197	ASP	N-CA-C	-6.83	94.17	107.62
1	A	275	ASN	N-CA-C	6.82	119.69	109.25
1	B	370	SER	N-CA-C	-6.80	100.72	110.59
1	A	19	MET	N-CA-C	6.78	120.43	111.75
1	B	312	ALA	CA-C-O	-6.76	114.22	121.45
1	A	52	VAL	N-CA-C	-6.75	103.90	110.72
1	A	169	LEU	N-CA-C	6.73	119.38	108.34
1	B	308	SER	CA-C-O	6.71	128.67	121.55
1	A	349	ALA	N-CA-C	-6.64	104.12	111.36
1	B	121	ALA	N-CA-C	-6.62	103.99	111.07
1	A	62	ILE	N-CA-C	6.62	120.15	113.47
1	A	370	SER	N-CA-C	-6.61	102.00	110.53
1	A	243	ALA	N-CA-C	-6.61	104.16	111.36
1	B	351	PHE	N-CA-C	6.60	122.27	111.37
1	B	169	LEU	N-CA-C	6.60	119.16	108.34
1	B	62	ILE	N-CA-C	6.59	119.49	113.10
1	B	176	VAL	N-CA-C	-6.58	98.15	107.75
1	A	51	ILE	CG1-CB-CG2	-6.58	90.97	110.70
1	A	115	THR	N-CA-C	-6.51	104.26	111.36
1	B	150	GLU	N-CA-C	6.50	122.36	113.77
1	A	310	ALA	N-CA-CB	6.49	120.13	110.40
1	A	293	THR	N-CA-C	6.47	119.15	111.71
1	B	380	SER	N-CA-C	-6.47	99.67	109.95
1	B	161	LEU	N-CA-C	-6.46	98.20	108.73
1	A	265	GLU	OE1-CD-OE2	-6.38	107.58	122.90
1	B	65	LYS	CA-C-N	6.31	129.25	120.29
1	B	65	LYS	C-N-CA	6.31	129.25	120.29
1	B	306	TYR	O-C-N	6.22	130.86	123.27
1	B	356	ASP	N-CA-C	-6.21	98.41	108.41
1	A	312	ALA	CA-C-N	-6.20	109.73	121.63
1	A	312	ALA	C-N-CA	-6.20	109.73	121.63
1	A	345	ALA	N-CA-C	-6.19	104.22	110.97
1	A	312	ALA	O-C-N	6.18	130.40	123.48
1	B	69	GLU	OE1-CD-OE2	6.16	137.69	122.90
1	B	244	LEU	N-CA-C	-6.16	104.49	111.14
1	B	167	ARG	N-CA-C	6.14	120.77	113.28
1	B	267	ILE	N-CA-C	6.14	118.06	112.29
1	B	129	PRO	N-CA-C	6.13	125.09	112.47
1	B	265	GLU	OE1-CD-OE2	-6.07	108.34	122.90
1	A	203	GLU	N-CA-C	6.00	117.82	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	SER	N-CA-C	5.99	118.28	110.43
1	A	108	LYS	N-CA-C	5.93	118.41	108.02
1	A	69	GLU	OE1-CD-OE2	5.93	137.14	122.90
1	A	195	MET	N-CA-C	-5.93	99.62	109.46
1	B	311	VAL	N-CA-CB	-5.92	102.53	112.47
1	B	92	LEU	N-CA-C	-5.85	104.81	111.07
1	A	129	PRO	N-CA-C	5.82	124.46	112.47
1	A	75	ILE	N-CA-C	5.78	116.44	108.12
1	A	338	ASN	N-CA-C	5.76	120.30	113.16
1	A	288	LEU	N-CA-C	-5.72	105.04	111.28
1	B	141	ALA	N-CA-C	5.69	118.33	107.75
1	B	349	ALA	N-CA-C	-5.68	105.00	111.14
1	A	149	GLY	N-CA-C	5.65	120.89	114.67
1	B	249	SER	N-CA-C	5.64	117.43	111.28
1	B	183	TYR	N-CA-C	5.63	118.06	109.62
1	B	239	MET	N-CA-C	5.57	117.03	111.07
1	B	294	THR	N-CA-C	5.56	119.90	113.18
1	B	337	ASP	N-CA-C	5.53	118.24	111.82
1	B	202	ASN	CB-CG-ND2	5.51	124.67	116.40
1	A	265	GLU	CG-CD-OE1	5.50	131.05	118.40
1	B	316	THR	N-CA-C	5.50	118.52	109.72
1	A	81	SER	N-CA-C	5.49	117.63	110.43
1	B	175	ASN	CA-C-N	-5.48	115.81	123.10
1	B	175	ASN	C-N-CA	-5.48	115.81	123.10
1	A	208	SER	N-CA-C	-5.47	105.21	111.07
1	A	262	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	A	66	GLU	N-CA-C	-5.43	105.52	111.82
1	A	202	ASN	CB-CG-ND2	5.42	124.53	116.40
1	A	173	GLU	CA-CB-CG	5.41	124.92	114.10
1	A	176	VAL	N-CA-C	-5.40	99.87	107.75
1	B	288	LEU	N-CA-C	-5.37	105.32	111.07
1	A	240	GLY	N-CA-C	-5.37	106.17	113.37
1	B	276	LEU	N-CA-C	-5.36	105.97	112.88
1	A	191	HIS	ND1-CG-CD2	-5.35	100.75	106.10
1	A	355	LEU	N-CA-C	-5.35	98.52	107.99
1	B	216	HIS	N-CA-C	-5.34	105.54	111.36
1	B	265	GLU	CG-CD-OE1	5.33	130.65	118.40
1	B	126	ALA	N-CA-C	-5.32	105.48	111.28
1	B	137	ALA	N-CA-C	-5.32	100.58	109.24
1	B	245	LEU	N-CA-C	5.32	117.07	111.28
1	B	360	ASP	N-CA-C	-5.31	101.82	110.20
1	A	350	MET	N-CA-C	5.30	117.14	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	PHE	N-CA-C	5.29	117.80	111.71
1	B	191	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	B	310	ALA	CA-C-N	-5.29	113.84	122.57
1	B	310	ALA	C-N-CA	-5.29	113.84	122.57
1	B	108	LYS	N-CA-C	5.28	117.27	108.02
1	B	196	VAL	CB-CA-C	-5.23	103.36	110.42
1	B	280	SER	N-CA-C	5.23	117.39	111.11
1	A	176	VAL	N-CA-CB	5.21	118.42	111.64
1	A	269	TYR	N-CA-C	-5.21	105.68	111.36
1	A	113	GLY	N-CA-C	5.21	125.53	113.18
1	A	337	ASP	N-CA-C	5.19	117.68	111.71
1	B	227	TYR	N-CA-C	5.19	117.42	109.07
1	A	5	ILE	N-CA-C	5.17	115.67	108.84
1	A	120	LEU	N-CA-C	-5.17	105.73	111.36
1	B	51	ILE	CB-CG1-CD1	-5.16	102.97	113.80
1	A	309	GLY	O-C-N	-5.14	117.94	122.77
1	A	202	ASN	CB-CA-C	-5.14	103.05	110.96
1	B	309	GLY	O-C-N	5.12	128.09	122.56
1	A	130	ASP	N-CA-C	-5.09	107.07	113.28
1	A	273	VAL	N-CA-C	5.06	119.87	109.34
1	A	191	HIS	CB-CA-C	-5.06	104.26	110.08
1	A	380	SER	N-CA-C	-5.06	101.91	109.95
1	B	275	ASN	N-CA-C	5.05	117.02	109.59
1	B	114	ALA	N-CA-C	-5.05	105.85	111.36
1	A	234	ILE	CA-C-N	-5.03	113.55	119.84
1	A	234	ILE	C-N-CA	-5.03	113.55	119.84

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	81	0
1	B	2969	0	2929	72	0
2	A	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
3	A	83	0	0	7	0
3	B	87	0	0	2	0
All	All	6128	0	5858	150	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 13.

All (150) 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:B:47:ILE:HD11	1:B:353:GLU:CD	2.03	0.84
1:A:59:ALA:HB3	1:A:96:MET:HE2	1.59	0.82
1:A:290:GLU:HB3	1:A:329:LYS:HG3	1.60	0.82
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:60:GLU:HA	1:B:96:MET:HE1	1.71	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:60:GLU:N	1:A:96:MET:HE1	2.09	0.67
1:A:309:GLY:N	1:A:310:ALA:HA	2.10	0.65
1:A:29:ASP:O	1:A:30:PRO:C	2.40	0.65
1:B:309:GLY:N	1:B:310:ALA:HA	2.12	0.64
1:B:42:MET:HE1	1:B:153:GLN:HE21	1.61	0.64
1:A:212:VAL:CG1	1:A:314:PHE:HB2	2.28	0.64
1:B:42:MET:HE3	1:B:153:GLN:HB2	1.79	0.63
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:B:308:SER:C	1:B:309:GLY:CA	2.71	0.62
1:A:177:MET:HE3	3:A:452:HOH:O	1.99	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:HE1	3:A:468:HOH:O	1.85	0.60
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:63:LEU:HD12	1:B:96:MET:HE3	1.85	0.58
1:A:329:LYS:O	1:A:332:HIS:N	2.37	0.57
1:B:362:THR:HG22	1:B:363:LEU:N	2.20	0.57
1:A:143:TYR:HE2	3:A:467:HOH:O	1.86	0.56
1:A:328:GLN:O	1:A:329:LYS:C	2.48	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
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:A:19:MET:HE3	1:A:42:MET:HB2	1.90	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:63:LEU:HD12	1:A:96:MET:HE3	1.90	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:60:GLU:CA	1:A:96:MET:HE1	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: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:308:SER:C	1:A:310:ALA:HA	2.35	0.52
1:A:47:ILE:HD11	1:A:353:GLU:CD	2.35	0.52
1:B:4:GLY:HA3	1:B:169:LEU:O	2.09	0.52
1:B:42:MET:HE1	1:B:153:GLN:NE2	2.25	0.51
1:B:5:ILE:HG21	1:B:8:ILE:CG2	2.41	0.51
1:B:308:SER:C	1:B:310:ALA:HA	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:202:ASN:HD21	1:A:239:MET:HE1	1.76	0.50
1:A:328:GLN:HB2	1:A:332:HIS:CE1	2.46	0.50
1:A:202:ASN:ND2	1:A:239:MET:HE1	2.25	0.49
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:B:42:MET:HE3	1:B:153:GLN:HE21	1.76	0.48
1:A:120:LEU:HD11	1:B:105:PHE:CZ	2.49	0.47
1:B:236:TYR:OH	1:B:239:MET:HE3	2.14	0.47
1:B:202:ASN:OD1	1:B:239:MET:HE1	2.15	0.47
1:A:269:TYR:O	1:A:273:VAL:HG23	2.15	0.47
1:A:59:ALA:HB3	1:A:96:MET:CE	2.39	0.47
1:B:60:GLU:CA	1:B:96:MET:HE1	2.41	0.47
1:B:180:GLN:O	1:B:310:ALA:N	2.47	0.47
1:B:42:MET:HE3	1:B:153:GLN:CB	2.43	0.46
1:A:29:ASP:C	1:A:31:GLY:N	2.72	0.46
1:B:5:ILE:HG21	1:B:8:ILE:HG23	1.96	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:A:236:TYR:OH	1:A:239:MET:HE3	2.15	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: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:59:ALA:CB	1:A:96:MET:HE2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:CYS:HB3	1:B:277:TYR:C	2.43	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:A:185:PHE:CD2	1:A:185:PHE:C	2.97	0.43
1:B:265:GLU:OE2	1:B:292:ALA:HA	2.19	0.42
1:A:290:GLU:CD	1:A:332:HIS:HD1	2.25	0.42
1:B:239:MET:HA	1:B:239:MET:HE2	2.01	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:B:185:PHE:C	1:B:185:PHE:CD2	2.98	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:B:14:PRO:HG2	1:B:15:TYR:CE2	2.55	0.42
1:A:112:TYR:CE2	1:A:311:VAL:HG11	2.55	0.41
1:A:66:GLU:H	1:A:66:GLU:CD	2.18	0.41
1:A:262:ARG:HD3	1:A:262:ARG:HH11	1.09	0.41
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

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	381/383 (100%)	365 (96%)	14 (4%)	2 (0%)	24	37
1	B	381/383 (100%)	367 (96%)	14 (4%)	0	100	100
All	All	762/766 (100%)	732 (96%)	28 (4%)	2 (0%)	36	50

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%)	284 (91%)	28 (9%)	9	15
1	B	312/312 (100%)	285 (91%)	27 (9%)	9	16
All	All	624/624 (100%)	569 (91%)	55 (9%)	9	15

All (55) 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	47	ILE

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Mol	Chain	Res	Type
1	A	65	LYS
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	212	VAL
1	A	237	THR
1	A	244	LEU
1	A	262	ARG
1	A	270	SER
1	A	288	LEU
1	A	294	THR
1	A	301	ILE
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
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	212	VAL
1	B	217	LYS
1	B	237	THR
1	B	244	LEU
1	B	247	LYS
1	B	262	ARG
1	B	270	SER

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Mol	Chain	Res	Type
1	B	288	LEU
1	B	294	THR
1	B	301	ILE
1	B	324	GLN
1	B	333	LEU
1	B	335	LEU
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	45	ASN
1	A	128	HIS
1	A	191	HIS
1	A	202	ASN
1	A	324	GLN
1	A	328	GLN
1	A	338	ASN
1	A	376	ASN
1	B	39	GLN
1	B	128	HIS
1	B	326	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 [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, 95th 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 ²)	Q<0.9
1	A	383/383 (100%)	0.29	11 (2%) 53 50	9, 18, 29, 38	0
1	B	383/383 (100%)	0.32	12 (3%) 51 47	9, 19, 29, 38	0
All	All	766/766 (100%)	0.31	23 (3%) 52 48	9, 18, 29, 38	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	ASN	3.7
1	B	309	GLY	3.6
1	A	309	GLY	3.6
1	A	364	GLU	3.1
1	A	203	GLU	2.9
1	A	30	PRO	2.8
1	A	190	GLY	2.7
1	B	69	GLU	2.6
1	A	383	ASN	2.5
1	B	165	GLU	2.4
1	A	65	LYS	2.4
1	B	298	GLY	2.3
1	B	355	LEU	2.3
1	B	37	ILE	2.2
1	A	253	GLU	2.2
1	B	375	ASN	2.1
1	A	354	THR	2.1
1	A	28	VAL	2.1
1	B	253	GLU	2.1
1	B	65	LYS	2.1
1	A	130	ASP	2.1
1	B	330	GLU	2.0
1	B	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 95th 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	SO4	A	384	5/5	0.91	0.12	45,45,46,47	0
2	SO4	A	385	5/5	0.91	0.14	15,15,15,15	5
2	SO4	B	385	5/5	0.92	0.16	44,45,47,47	0
2	SO4	B	384	5/5	0.93	0.18	12,13,13,13	5

6.5 Other polymers [i](#)

There are no such residues in this entry.