



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:26 PM UTC

PDB ID : 1VGW / pdb_00001vgw
Title : Crystal structure of 4-diphosphocytidyl-2C-methyl-D-erythritol synthase
Authors : Structural GenomiX
Deposited on : 2003-11-03
Resolution : 2.35 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
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

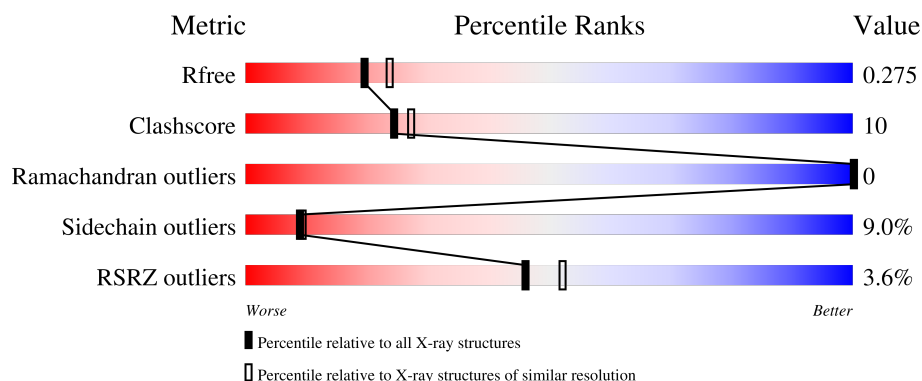
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	231	5% 72% 16% • 8%
1	B	231	4% 71% 17% • 7%
1	C	231	3% 69% 21% • 7%
1	D	231	2% 71% 18% • 9%
1	E	231	3% 70% 19% • 8%

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Mol	Chain	Length	Quality of chain
1	F	231	2% 68% 18% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9804 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 4-diphosphocytidyl-2C-methyl-D-erythritol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1584	994	289	299	2			
1	B	214	Total	C	N	O	S	0	0	0
			1609	1010	292	305	2			
1	C	214	Total	C	N	O	S	0	0	0
			1603	1007	290	304	2			
1	D	211	Total	C	N	O	S	0	0	0
			1587	996	287	302	2			
1	E	213	Total	C	N	O	S	0	0	0
			1595	1002	286	305	2			
1	F	209	Total	C	N	O	S	0	0	0
			1569	985	282	300	2			

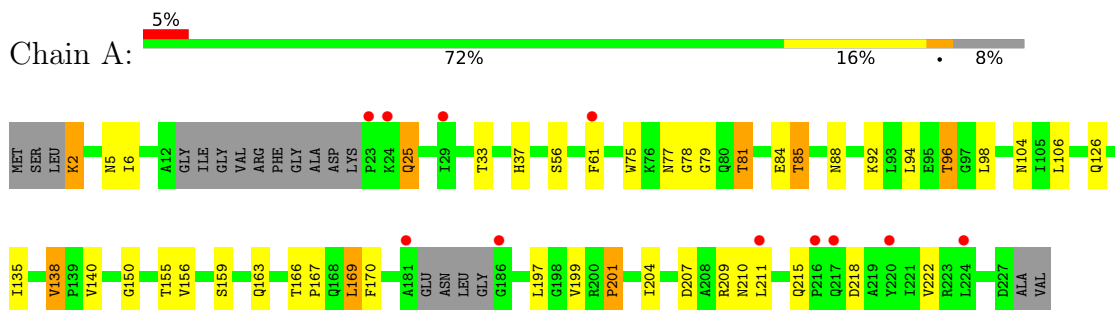
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total	O	0	0
			39	39		
2	B	59	Total	O	0	0
			59	59		
2	C	30	Total	O	0	0
			30	30		
2	D	38	Total	O	0	0
			38	38		
2	E	52	Total	O	0	0
			52	52		
2	F	39	Total	O	0	0
			39	39		

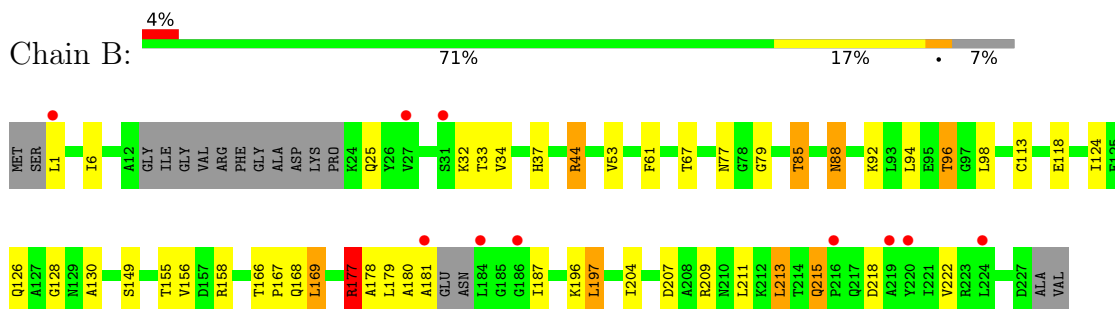
3 Residue-property plots [i](#)

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.

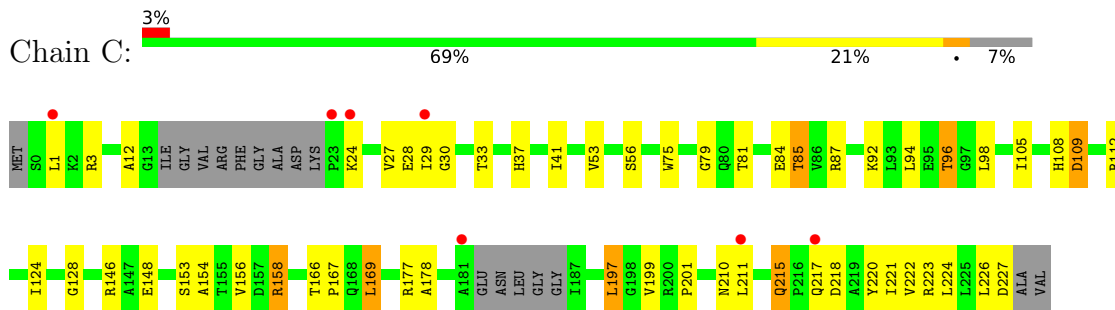
- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase



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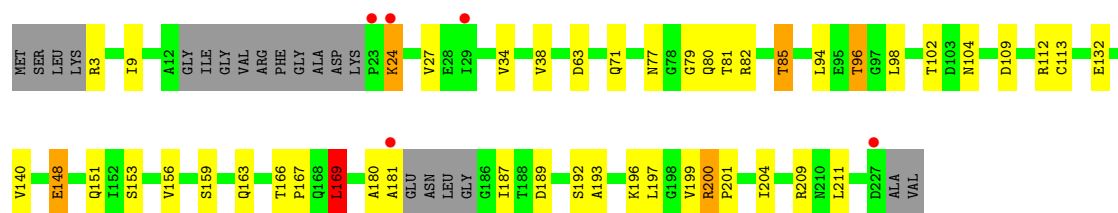


- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase

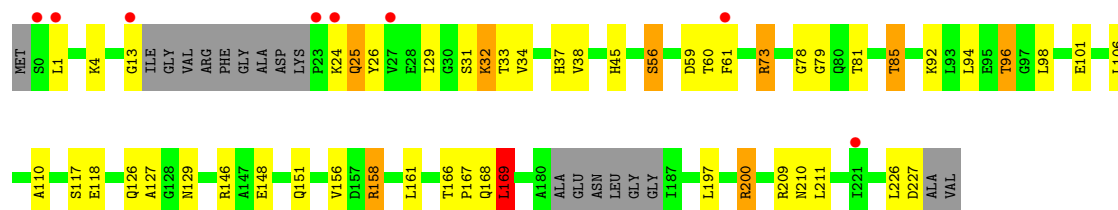


- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase

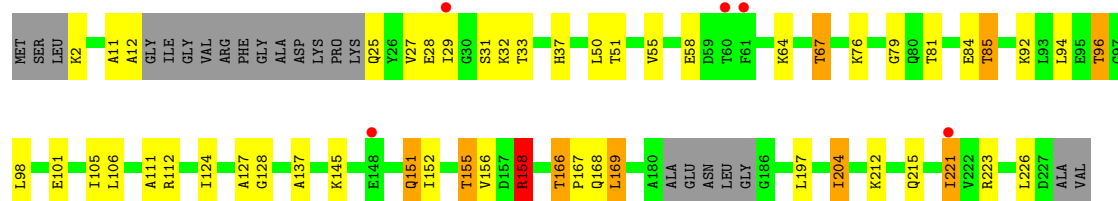




- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.17Å 95.11Å 173.86Å 90.00° 93.65° 90.00°	Depositor
Resolution (Å)	39.47 – 2.35 39.47 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.47-2.35) 99.9 (39.47-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.34Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.260 , 0.317 0.225 , 0.275	Depositor DCC
R_{free} test set	3449 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9804	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% 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

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	0.88	0/1603	1.49	8/2176 (0.4%)
1	B	0.90	0/1628	1.44	6/2209 (0.3%)
1	C	0.85	0/1622	1.47	11/2204 (0.5%)
1	D	0.83	0/1607	1.41	6/2183 (0.3%)
1	E	0.91	0/1615	1.57	15/2194 (0.7%)
1	F	0.90	1/1588 (0.1%)	1.45	9/2158 (0.4%)
All	All	0.87	1/9663 (0.0%)	1.47	55/13124 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	137	ALA	C-N	5.47	1.37	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	ARG	CD-NE-CZ	13.39	143.14	124.40
1	F	137	ALA	CA-C-N	-8.06	116.31	123.33
1	F	137	ALA	C-N-CA	-8.06	116.31	123.33
1	E	200	ARG	CA-C-N	6.88	126.84	119.76
1	E	200	ARG	C-N-CA	6.88	126.84	119.76
1	C	109	ASP	CA-CB-CG	6.72	119.32	112.60
1	C	30	GLY	N-CA-C	-6.71	103.20	111.45
1	E	169	LEU	N-CA-C	6.71	119.62	108.96
1	D	200	ARG	CD-NE-CZ	6.41	133.37	124.40
1	A	138	VAL	CA-C-O	6.38	123.47	119.51
1	A	135	ILE	CA-C-O	-6.31	115.05	121.67
1	E	148	GLU	CA-C-O	-6.30	115.70	119.55
1	E	24	LYS	N-CA-C	6.19	119.01	110.35
1	A	25	GLN	N-CA-C	-6.08	105.51	113.17
1	D	24	LYS	N-CA-C	6.04	119.70	112.93
1	C	177	ARG	CG-CD-NE	5.97	125.14	112.00
1	E	129	ASN	CA-CB-CG	-5.82	106.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	ASN	CA-CB-CG	5.80	118.40	112.60
1	E	45	HIS	CA-C-N	5.74	127.97	120.28
1	E	45	HIS	C-N-CA	5.74	127.97	120.28
1	C	210	ASN	CA-CB-CG	5.73	118.33	112.60
1	E	210	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	F	127	ALA	CA-C-N	5.67	127.23	120.14
1	F	127	ALA	C-N-CA	5.67	127.23	120.14
1	D	169	LEU	N-CA-C	5.66	117.51	108.41
1	E	168	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	E	25	GLN	N-CA-C	-5.55	106.18	113.17
1	D	189	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	6	ILE	N-CA-C	5.54	115.83	107.80
1	E	169	LEU	CA-CB-CG	5.52	135.63	116.30
1	F	112	ARG	CD-NE-CZ	-5.49	116.71	124.40
1	F	168	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	177	ARG	CD-NE-CZ	5.43	132.00	124.40
1	B	53	VAL	CA-C-O	-5.38	114.74	120.39
1	A	170	PHE	O-C-N	-5.35	117.06	123.27
1	B	168	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	C	53	VAL	CA-C-O	-5.32	114.72	120.36
1	A	150	GLY	N-CA-C	-5.32	107.34	115.00
1	E	73	ARG	CD-NE-CZ	-5.31	116.97	124.40
1	C	105	ILE	CA-C-N	5.27	130.18	122.85
1	C	105	ILE	C-N-CA	5.27	130.18	122.85
1	E	127	ALA	CA-C-O	5.24	124.59	118.77
1	E	126	GLN	CA-C-O	-5.20	113.18	119.27
1	D	9	ILE	N-CA-C	5.20	113.17	107.60
1	F	166	THR	CA-C-O	-5.19	115.50	120.64
1	B	130	ALA	CA-C-O	-5.19	114.76	120.36
1	C	215	GLN	CA-C-N	5.17	125.21	119.32
1	C	215	GLN	C-N-CA	5.17	125.21	119.32
1	D	71	GLN	N-CA-C	5.15	119.55	113.16
1	B	6	ILE	N-CA-C	5.06	115.14	107.75
1	F	204	ILE	O-C-N	-5.06	117.98	123.14
1	C	41	ILE	O-C-N	-5.05	116.96	121.91
1	A	201	PRO	CA-C-O	-5.02	115.55	121.67
1	A	210	ASN	CA-CB-CG	5.01	117.61	112.60
1	F	158	ARG	CD-NE-CZ	5.01	131.41	124.40

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	1584	0	1622	36	0
1	B	1609	0	1650	32	1
1	C	1603	0	1637	35	0
1	D	1587	0	1617	28	0
1	E	1595	0	1619	30	1
1	F	1569	0	1593	33	0
2	A	39	0	0	0	0
2	B	59	0	0	2	0
2	C	30	0	0	2	0
2	D	38	0	0	1	0
2	E	52	0	0	2	0
2	F	39	0	0	4	0
All	All	9804	0	9738	190	1

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 10.

All (190) 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:C:79:GLY:H	1:C:85:THR:HG22	1.24	0.97
1:F:79:GLY:H	1:F:85:THR:HG22	1.28	0.95
1:E:79:GLY:H	1:E:85:THR:HG22	1.32	0.94
1:C:84:GLU:HG3	1:C:87:ARG:NH2	1.87	0.89
1:A:79:GLY:H	1:A:85:THR:HG22	1.44	0.80
1:B:79:GLY:H	1:B:85:THR:HG22	1.47	0.80
1:D:3:ARG:HD3	1:D:102:THR:O	1.82	0.79
1:B:44:ARG:HH11	1:B:44:ARG:HB3	1.50	0.77
1:C:79:GLY:N	1:C:85:THR:HG22	2.01	0.74
1:F:96:THR:HG22	1:F:98:LEU:H	1.52	0.74
1:A:211:LEU:HD11	1:A:222:VAL:HG23	1.73	0.70
1:A:96:THR:CG2	1:A:98:LEU:H	2.05	0.70
1:E:158:ARG:HG3	1:E:158:ARG:HH21	1.57	0.70
1:A:77:ASN:HD22	1:A:88:ASN:HB3	1.57	0.68
1:B:180:ALA:O	1:B:181:ALA:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG12	1:C:29:ILE:HG13	1.75	0.68
1:C:226:LEU:O	1:C:227:ASP:HB2	1.93	0.68
1:A:33:THR:HG21	1:A:61:PHE:HE2	1.58	0.68
1:E:92:LYS:O	1:E:96:THR:HB	1.92	0.68
1:E:96:THR:HG22	1:E:98:LEU:H	1.60	0.67
1:F:79:GLY:N	1:F:85:THR:HG22	2.08	0.67
1:B:44:ARG:HB3	1:B:44:ARG:NH1	2.09	0.67
1:A:92:LYS:O	1:A:96:THR:HB	1.95	0.66
1:E:209:ARG:HD2	2:E:276:HOH:O	1.95	0.65
1:A:126:GLN:HE21	1:A:204:ILE:HG12	1.59	0.65
1:F:145:LYS:HG3	1:F:152:ILE:HD13	1.76	0.65
1:A:207:ASP:OD2	1:A:209:ARG:HD3	1.97	0.65
1:D:148:GLU:HB2	1:D:153:SER:HB3	1.80	0.64
1:C:84:GLU:HG3	1:C:87:ARG:HH22	1.62	0.64
1:A:166:THR:HB	1:A:167:PRO:HA	1.80	0.62
1:F:101:GLU:HG2	2:F:238:HOH:O	1.99	0.62
1:C:27:VAL:O	1:C:33:THR:HA	2.01	0.61
1:F:96:THR:HG21	1:F:98:LEU:HD12	1.83	0.61
1:C:81:THR:OG1	1:C:84:GLU:HB2	2.01	0.61
1:B:207:ASP:OD2	1:B:209:ARG:HD3	2.02	0.60
1:E:79:GLY:H	1:E:85:THR:CG2	2.11	0.60
1:E:166:THR:HB	1:E:167:PRO:HA	1.84	0.60
1:A:96:THR:HG23	1:A:98:LEU:H	1.66	0.60
1:A:126:GLN:NE2	1:A:204:ILE:HG12	2.16	0.60
1:B:215:GLN:HG2	1:B:218:ASP:OD1	2.02	0.60
1:F:215:GLN:HG2	2:F:234:HOH:O	2.03	0.59
1:E:96:THR:HG21	1:E:98:LEU:HD12	1.85	0.58
1:B:44:ARG:HH11	1:B:44:ARG:CB	2.15	0.58
1:B:79:GLY:H	1:B:85:THR:CG2	2.15	0.58
1:D:104:ASN:HB3	1:D:169:LEU:HD13	1.86	0.58
1:A:96:THR:HG21	1:A:98:LEU:HD12	1.86	0.57
1:C:29:ILE:HG23	1:C:223:ARG:HD2	1.86	0.57
1:A:81:THR:HG23	1:A:84:GLU:H	1.70	0.57
1:F:81:THR:OG1	1:F:84:GLU:HB2	2.04	0.57
1:B:92:LYS:O	1:B:96:THR:HB	2.04	0.57
1:A:211:LEU:HD11	1:A:222:VAL:CG2	2.34	0.57
1:E:79:GLY:N	1:E:85:THR:HG22	2.13	0.56
1:C:75:TRP:CE3	1:C:92:LYS:HD3	2.40	0.56
1:A:81:THR:HG23	1:A:84:GLU:HB2	1.86	0.56
1:D:166:THR:HB	1:D:167:PRO:HA	1.88	0.56
1:A:33:THR:HG21	1:A:61:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:THR:HG22	1:F:98:LEU:N	2.20	0.56
1:E:226:LEU:O	1:E:227:ASP:HB2	2.06	0.55
1:B:77:ASN:HD22	1:B:88:ASN:HB3	1.72	0.55
1:E:25:GLN:O	1:E:34:VAL:HB	2.07	0.55
1:C:211:LEU:HD11	1:C:222:VAL:CG2	2.37	0.54
1:F:28:GLU:HG2	1:F:33:THR:HG22	1.89	0.54
1:D:34:VAL:O	1:D:38:VAL:HG23	2.08	0.54
1:B:96:THR:HG22	1:B:98:LEU:H	1.73	0.54
1:F:79:GLY:H	1:F:85:THR:CG2	2.12	0.54
1:B:96:THR:CG2	1:B:98:LEU:HG	2.38	0.53
1:A:96:THR:HG22	1:A:98:LEU:H	1.73	0.53
1:B:166:THR:HB	1:B:167:PRO:HA	1.91	0.53
1:C:96:THR:HG21	1:C:98:LEU:HD12	1.90	0.53
1:F:92:LYS:O	1:F:96:THR:HB	2.09	0.52
1:A:106:LEU:HD11	1:A:169:LEU:HD22	1.91	0.52
1:D:180:ALA:O	1:D:181:ALA:CB	2.57	0.52
1:F:166:THR:HB	1:F:167:PRO:HA	1.92	0.51
1:C:153:SER:O	1:C:154:ALA:HB2	2.11	0.51
1:D:109:ASP:HB2	1:D:112:ARG:HG3	1.92	0.51
1:A:78:GLY:HA2	1:A:85:THR:HB	1.92	0.51
1:A:75:TRP:CE2	1:A:92:LYS:HE2	2.45	0.51
1:C:199:VAL:O	1:C:201:PRO:HD3	2.11	0.51
1:F:64:LYS:O	1:F:67:THR:HB	2.11	0.51
1:B:96:THR:HG21	1:B:98:LEU:HD12	1.94	0.50
1:F:106:LEU:HG	1:F:169:LEU:HB2	1.92	0.50
1:E:81:THR:O	1:E:85:THR:HG23	2.11	0.50
1:A:215:GLN:HG2	1:A:218:ASP:OD1	2.11	0.50
1:E:200:ARG:HG2	1:F:152:ILE:O	2.12	0.50
1:B:213:LEU:C	1:B:213:LEU:HD12	2.37	0.50
1:A:2:LYS:HG2	1:D:200:ARG:HH22	1.75	0.50
1:C:96:THR:HG23	1:C:98:LEU:HG	1.94	0.49
1:A:79:GLY:H	1:A:85:THR:CG2	2.20	0.49
1:B:118:GLU:HB2	2:B:259:HOH:O	2.10	0.49
1:C:178:ALA:HB2	1:C:197:LEU:HD22	1.93	0.49
1:B:33:THR:HG21	1:B:61:PHE:CE2	2.48	0.49
1:D:169:LEU:C	1:D:169:LEU:HD12	2.38	0.49
1:F:11:ALA:HB1	1:F:25:GLN:NE2	2.28	0.49
1:A:81:THR:O	1:A:85:THR:HG23	2.12	0.49
1:E:13:GLY:H	1:E:56:SER:HB3	1.78	0.49
1:E:226:LEU:O	1:E:227:ASP:CB	2.61	0.48
1:D:187:ILE:HD13	1:D:193:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LEU:HD12	1:B:169:LEU:C	2.38	0.48
1:D:209:ARG:O	1:D:211:LEU:HD23	2.13	0.48
1:D:3:ARG:HB3	2:D:257:HOH:O	2.14	0.48
1:F:151:GLN:NE2	2:F:263:HOH:O	2.46	0.48
1:B:124:ILE:O	1:B:128:GLY:HA3	2.12	0.48
1:C:37:HIS:CD2	1:C:226:LEU:HD13	2.49	0.48
1:E:37:HIS:ND1	2:E:278:HOH:O	2.35	0.47
1:F:106:LEU:HD11	1:F:169:LEU:HD22	1.96	0.47
1:F:158:ARG:HD2	2:F:244:HOH:O	2.14	0.47
1:D:199:VAL:O	1:D:201:PRO:HD3	2.15	0.47
1:B:180:ALA:O	1:B:181:ALA:CB	2.58	0.47
1:E:158:ARG:HA	1:E:161:LEU:HD12	1.96	0.47
1:F:29:ILE:HG23	1:F:223:ARG:CZ	2.44	0.47
1:C:211:LEU:HD12	1:C:211:LEU:O	2.14	0.47
1:B:169:LEU:C	1:B:169:LEU:CD1	2.88	0.46
1:E:78:GLY:HA2	1:E:85:THR:HB	1.96	0.46
1:C:211:LEU:HD12	1:C:211:LEU:C	2.40	0.46
1:A:79:GLY:N	1:A:85:THR:HG22	2.19	0.46
1:A:25:GLN:H	1:A:25:GLN:HG2	1.58	0.46
1:C:169:LEU:C	1:C:169:LEU:HD12	2.41	0.46
1:C:215:GLN:HG2	1:C:218:ASP:OD1	2.16	0.46
1:E:158:ARG:HH21	1:E:158:ARG:CG	2.20	0.46
1:E:38:VAL:HG21	1:E:110:ALA:O	2.16	0.46
1:F:111:ALA:HB3	1:F:212:LYS:HG3	1.97	0.46
1:B:34:VAL:HG13	1:B:113:CYS:SG	2.56	0.46
1:B:169:LEU:HD12	1:B:169:LEU:O	2.16	0.46
1:B:218:ASP:O	1:B:222:VAL:HG23	2.15	0.45
1:D:82:ARG:HG2	1:D:82:ARG:HH21	1.79	0.45
1:F:12:ALA:HB3	1:F:85:THR:HG21	1.97	0.45
1:B:187:ILE:HG22	1:B:196:LYS:HE3	1.99	0.45
1:D:96:THR:CG2	1:D:98:LEU:H	2.30	0.45
1:D:140:VAL:HG22	1:D:163:GLN:HG3	1.99	0.45
1:E:26:TYR:OH	1:E:59:ASP:OD1	2.31	0.45
1:B:179:LEU:HD13	2:B:263:HOH:O	2.17	0.45
1:F:145:LYS:NZ	1:F:155:THR:OG1	2.50	0.45
1:C:166:THR:HB	1:C:167:PRO:HA	1.97	0.45
1:D:24:LYS:HA	1:D:27:VAL:HG23	1.98	0.44
1:D:96:THR:HG21	1:D:98:LEU:HD12	2.00	0.44
1:F:124:ILE:O	1:F:128:GLY:HA3	2.17	0.44
1:D:79:GLY:H	1:D:85:THR:HG22	1.82	0.44
1:C:211:LEU:HD11	1:C:222:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ILE:HD11	1:D:209:ARG:HG3	1.98	0.44
1:B:187:ILE:HG22	1:B:196:LYS:CE	2.48	0.44
1:E:73:ARG:HH11	1:E:73:ARG:HD2	1.55	0.44
1:F:221:ILE:H	1:F:221:ILE:HG13	1.60	0.43
1:D:211:LEU:HD23	1:D:211:LEU:H	1.83	0.43
1:B:178:ALA:HB2	1:B:197:LEU:HD22	2.00	0.43
1:C:220:TYR:O	1:C:224:LEU:HB2	2.19	0.43
1:F:106:LEU:CD1	1:F:169:LEU:HD22	2.48	0.43
1:A:81:THR:HG23	1:A:84:GLU:CB	2.48	0.43
1:F:2:LYS:HE2	1:F:2:LYS:HB2	1.90	0.43
1:A:211:LEU:HD12	1:A:211:LEU:C	2.43	0.43
1:E:32:LYS:HE2	1:E:37:HIS:CE1	2.54	0.43
1:A:140:VAL:HG22	1:A:163:GLN:HG3	2.00	0.43
1:F:50:LEU:HG	1:F:51:THR:N	2.33	0.43
1:C:96:THR:CG2	1:C:98:LEU:H	2.32	0.43
1:C:226:LEU:O	1:C:227:ASP:CB	2.62	0.43
1:D:180:ALA:O	1:D:181:ALA:HB3	2.18	0.43
1:D:132:GLU:HB2	1:D:199:VAL:CG1	2.49	0.42
1:A:106:LEU:CD1	1:A:169:LEU:HD22	2.49	0.42
1:F:169:LEU:C	1:F:169:LEU:HD12	2.45	0.42
1:C:12:ALA:HB3	1:C:85:THR:HG21	2.02	0.42
1:E:211:LEU:HD12	1:E:211:LEU:O	2.19	0.42
1:C:158:ARG:HH21	1:C:158:ARG:HG3	1.84	0.42
1:D:192:SER:O	1:D:196:LYS:HG3	2.20	0.42
1:A:75:TRP:CE3	1:A:92:LYS:HD3	2.55	0.42
1:E:158:ARG:CG	1:E:158:ARG:NH2	2.80	0.42
1:F:55:VAL:CG2	1:F:76:LYS:HG2	2.50	0.42
1:C:146:ARG:HH21	1:C:146:ARG:HD2	1.64	0.42
1:B:215:GLN:HG2	1:B:218:ASP:CG	2.44	0.41
1:D:79:GLY:H	1:D:85:THR:HB	1.85	0.41
1:B:32:LYS:HE2	1:B:37:HIS:CE1	2.55	0.41
1:D:96:THR:HG23	1:D:98:LEU:H	1.85	0.41
1:C:3:ARG:HG2	2:C:256:HOH:O	2.20	0.41
1:A:199:VAL:O	1:A:201:PRO:HD3	2.20	0.41
1:D:34:VAL:HG13	1:D:113:CYS:SG	2.60	0.41
1:C:109:ASP:HB2	1:C:112:ARG:HG3	2.03	0.41
1:E:33:THR:HG21	1:E:61:PHE:CE2	2.55	0.41
1:E:106:LEU:HD11	1:E:169:LEU:HD22	2.03	0.41
1:A:169:LEU:HD12	1:A:169:LEU:C	2.46	0.41
1:B:126:GLN:HE21	1:B:204:ILE:HG12	1.86	0.41
1:E:146:ARG:HG3	1:E:146:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HG2	1:D:200:ARG:NH2	2.35	0.41
1:A:5:ASN:OD1	1:A:104:ASN:HB2	2.19	0.41
1:A:75:TRP:HB3	1:A:77:ASN:OD1	2.21	0.41
1:B:177:ARG:HE	1:B:177:ARG:HB2	1.66	0.41
1:C:108:HIS:HD1	1:C:167:PRO:HG3	1.87	0.41
1:C:124:ILE:O	1:C:128:GLY:HA3	2.20	0.41
1:E:26:TYR:CE2	1:E:61:PHE:HD2	2.39	0.41
1:F:33:THR:O	1:F:37:HIS:HD2	2.04	0.41
1:C:1:LEU:HD11	2:C:233:HOH:O	2.21	0.40
1:E:146:ARG:HG3	1:E:146:ARG:NH1	2.37	0.40
1:F:37:HIS:CE1	1:F:226:LEU:HD13	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:O	1:E:4:LYS:NZ[2_756]	2.16	0.04

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	206/231 (89%)	191 (93%)	15 (7%)	0	100	100
1	B	208/231 (90%)	198 (95%)	10 (5%)	0	100	100
1	C	208/231 (90%)	201 (97%)	7 (3%)	0	100	100
1	D	205/231 (89%)	195 (95%)	10 (5%)	0	100	100
1	E	207/231 (90%)	194 (94%)	13 (6%)	0	100	100
1	F	203/231 (88%)	197 (97%)	6 (3%)	0	100	100
All	All	1237/1386 (89%)	1176 (95%)	61 (5%)	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	163/180 (91%)	150 (92%)	13 (8%)	11	12
1	B	166/180 (92%)	150 (90%)	16 (10%)	8	7
1	C	165/180 (92%)	153 (93%)	12 (7%)	13	14
1	D	164/180 (91%)	150 (92%)	14 (8%)	10	11
1	E	164/180 (91%)	147 (90%)	17 (10%)	7	6
1	F	162/180 (90%)	145 (90%)	17 (10%)	6	6
All	All	984/1080 (91%)	895 (91%)	89 (9%)	9	9

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	37	HIS
1	A	56	SER
1	A	81	THR
1	A	85	THR
1	A	94	LEU
1	A	96	THR
1	A	138	VAL
1	A	155	THR
1	A	156	VAL
1	A	159	SER
1	A	169	LEU
1	A	197	LEU
1	B	1	LEU
1	B	25	GLN
1	B	44	ARG
1	B	85	THR
1	B	94	LEU
1	B	96	THR

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Mol	Chain	Res	Type
1	B	149	SER
1	B	155	THR
1	B	156	VAL
1	B	158	ARG
1	B	169	LEU
1	B	177	ARG
1	B	197	LEU
1	B	211	LEU
1	B	213	LEU
1	B	215	GLN
1	C	24	LYS
1	C	28	GLU
1	C	56	SER
1	C	85	THR
1	C	94	LEU
1	C	96	THR
1	C	148	GLU
1	C	156	VAL
1	C	158	ARG
1	C	169	LEU
1	C	197	LEU
1	C	217	GLN
1	D	63	ASP
1	D	77	ASN
1	D	80	GLN
1	D	81	THR
1	D	85	THR
1	D	94	LEU
1	D	96	THR
1	D	148	GLU
1	D	151	GLN
1	D	156	VAL
1	D	159	SER
1	D	169	LEU
1	D	197	LEU
1	D	204	ILE
1	E	1	LEU
1	E	29	ILE
1	E	31	SER
1	E	32	LYS
1	E	56	SER
1	E	60	THR

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Mol	Chain	Res	Type
1	E	85	THR
1	E	94	LEU
1	E	96	THR
1	E	101	GLU
1	E	117	SER
1	E	118	GLU
1	E	151	GLN
1	E	156	VAL
1	E	158	ARG
1	E	169	LEU
1	E	197	LEU
1	F	27	VAL
1	F	31	SER
1	F	32	LYS
1	F	58	GLU
1	F	67	THR
1	F	85	THR
1	F	94	LEU
1	F	96	THR
1	F	105	ILE
1	F	151	GLN
1	F	155	THR
1	F	156	VAL
1	F	158	ARG
1	F	169	LEU
1	F	197	LEU
1	F	204	ILE
1	F	221	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	80	GLN
1	A	126	GLN
1	A	163	GLN
1	B	25	GLN
1	B	80	GLN
1	B	88	ASN
1	B	126	GLN
1	B	151	GLN
1	B	171	GLN

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Mol	Chain	Res	Type
1	B	205	GLN
1	B	215	GLN
1	C	80	GLN
1	C	151	GLN
1	D	80	GLN
1	D	171	GLN
1	E	5	ASN
1	E	37	HIS
1	E	80	GLN
1	E	104	ASN
1	E	205	GLN
1	F	25	GLN
1	F	37	HIS
1	F	80	GLN
1	F	171	GLN

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 ⓘ

There are no ligands in this entry.

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, 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	212/231 (91%)	0.18	11 (5%)	33 38	22, 39, 76, 88	0
1	B	214/231 (92%)	0.16	10 (4%)	36 42	22, 38, 73, 84	0
1	C	214/231 (92%)	0.27	7 (3%)	49 56	25, 42, 71, 90	0
1	D	211/231 (91%)	0.31	5 (2%)	59 66	28, 43, 75, 84	0
1	E	213/231 (92%)	0.13	8 (3%)	44 50	23, 37, 70, 95	0
1	F	209/231 (90%)	0.10	5 (2%)	59 66	21, 38, 68, 82	0
All	All	1273/1386 (91%)	0.19	46 (3%)	46 52	21, 39, 74, 95	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	PRO	4.2
1	D	29	ILE	3.6
1	C	29	ILE	3.6
1	B	184	LEU	3.6
1	A	220	TYR	3.5
1	A	181	ALA	3.4
1	B	220	TYR	3.3
1	A	61	PHE	3.2
1	E	13	GLY	3.2
1	B	224	LEU	3.2
1	E	24	LYS	3.1
1	F	221	ILE	3.1
1	C	181	ALA	3.0
1	A	186	GLY	3.0
1	A	23	PRO	2.9
1	E	23	PRO	2.7
1	B	1	LEU	2.7
1	B	216	PRO	2.6
1	D	181	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	29	ILE	2.6
1	A	211	LEU	2.6
1	C	23	PRO	2.5
1	D	24	LYS	2.5
1	B	219	ALA	2.5
1	B	31	SER	2.4
1	E	61	PHE	2.4
1	A	217	GLN	2.4
1	A	216	PRO	2.4
1	C	211	LEU	2.4
1	D	227	ASP	2.3
1	B	181	ALA	2.3
1	C	24	LYS	2.3
1	F	61	PHE	2.2
1	A	224	LEU	2.2
1	C	1	LEU	2.2
1	B	27	VAL	2.2
1	E	27	VAL	2.2
1	B	186	GLY	2.2
1	E	1	LEU	2.2
1	E	221	ILE	2.2
1	F	29	ILE	2.2
1	A	24	LYS	2.2
1	E	0	SER	2.1
1	C	217	GLN	2.1
1	F	60	THR	2.1
1	F	148	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.