



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:33 am BST

PDB ID : 1VGW
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

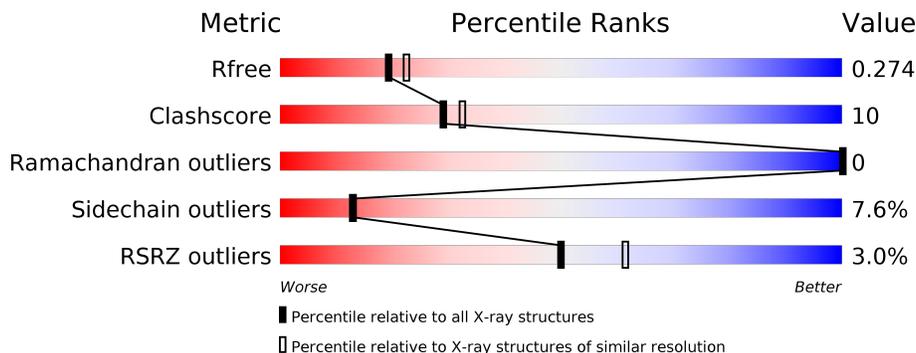
1 Overall quality at a glance i

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 on 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 74% 15% • 8%</p>
1	B	231	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 72% 16% •• 7%</p>
1	C	231	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 71% 18% •• 7%</p>
1	D	231	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 72% 16% •• 9%</p>
1	E	231	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 73% 17% •• 8%</p>
1	F	231	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 70% 18% •• 10%</p>

2 Entry composition [i](#)

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

- Molecule 2 is water.

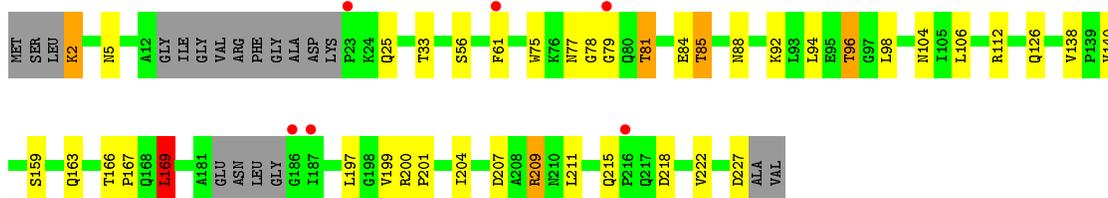
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total 39	O 39	0	0
2	B	59	Total 59	O 59	0	0
2	C	30	Total 30	O 30	0	0
2	D	38	Total 38	O 38	0	0
2	E	52	Total 52	O 52	0	0
2	F	39	Total 39	O 39	0	0

3 Residue-property plots [i](#)

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

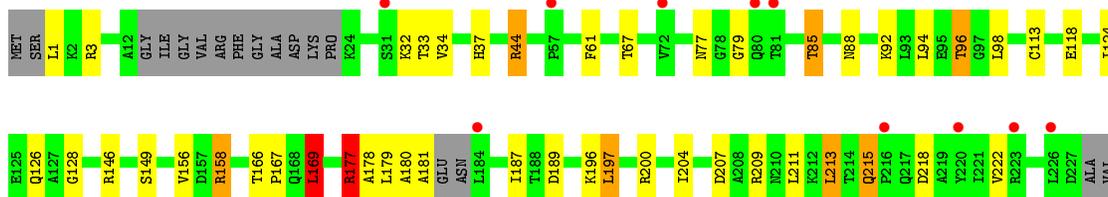
- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase

Chain A: 



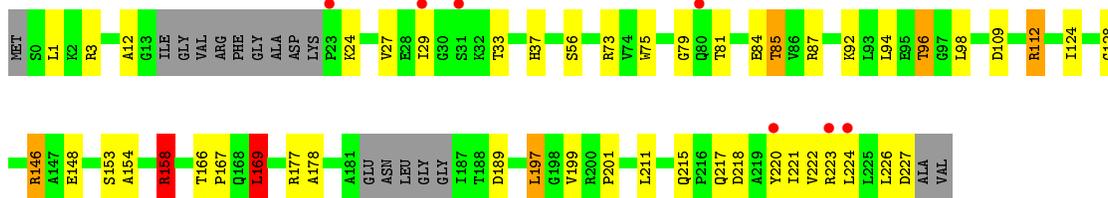
- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase

Chain B: 



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

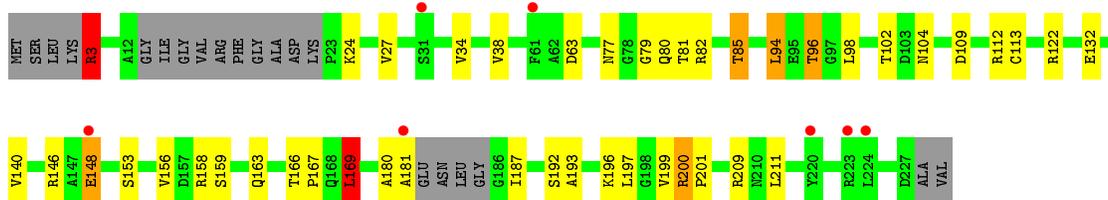
Chain C: 



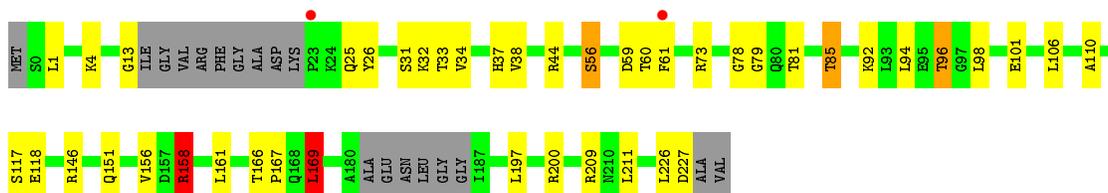
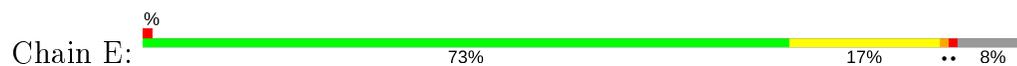
- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase

Chain D: 

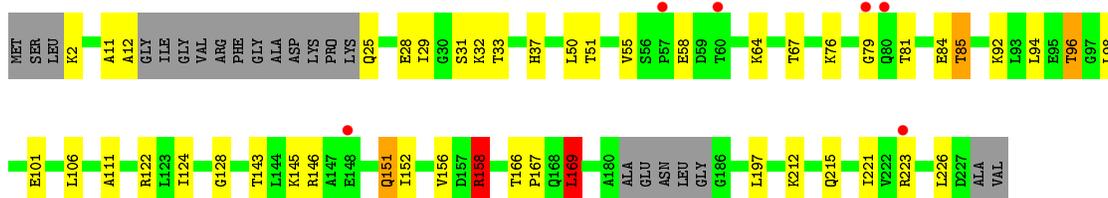




- Molecule 1: 4-diphosphocytidyl-2C-methyl-D-erythritol synthase



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



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)	Xtrriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.260 , 0.317 0.225 , 0.274	Depositor DCC
R_{free} test set	3449 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtrriage
Anisotropy	0.534	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9804	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage'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	0.66	0/1603	1.10	5/2176 (0.2%)
1	B	0.68	0/1628	1.15	7/2209 (0.3%)
1	C	0.64	0/1622	1.15	9/2204 (0.4%)
1	D	0.62	0/1607	1.05	7/2183 (0.3%)
1	E	0.67	0/1615	1.18	5/2194 (0.2%)
1	F	0.67	0/1588	1.06	4/2158 (0.2%)
All	All	0.66	0/9663	1.12	37/13124 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	ARG	CD-NE-CZ	13.96	143.14	123.60
1	E	158	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	D	200	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	E	169	LEU	CA-CB-CG	8.84	135.63	115.30
1	C	177	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	E	158	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	112	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	F	169	LEU	CA-CB-CG	7.01	131.42	115.30
1	D	200	ARG	CD-NE-CZ	6.98	133.37	123.60
1	C	169	LEU	CA-CB-CG	6.89	131.16	115.30
1	C	112	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	E	44	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	B	189	ASP	CB-CG-OD1	6.63	124.26	118.30
1	A	169	LEU	CA-CB-CG	6.48	130.21	115.30
1	D	169	LEU	CA-CB-CG	6.46	130.16	115.30
1	C	177	ARG	CG-CD-NE	6.35	125.14	111.80
1	B	169	LEU	CA-CB-CG	6.29	129.76	115.30
1	B	177	ARG	CD-NE-CZ	6.00	132.00	123.60
1	B	158	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	3	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	F	146	ARG	NE-CZ-NH1	5.92	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	B	146	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	F	158	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	200	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	200	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	146	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	209	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	C	73	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	94	LEU	CA-CB-CG	5.39	127.69	115.30
1	F	122	ARG	CD-NE-CZ	5.38	131.13	123.60
1	A	169	LEU	CB-CG-CD1	5.37	120.14	111.00
1	C	158	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	122	ARG	CD-NE-CZ	5.22	130.91	123.60
1	C	189	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	3	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	E	169	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	34	0
1	B	1609	0	1650	31	1
1	C	1603	0	1637	34	0
1	D	1587	0	1617	28	0
1	E	1595	0	1619	30	1
1	F	1569	0	1593	32	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	185	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 (185) 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:HB3	1:B:44:ARG:HH11	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:HH21	1:E:158:ARG:HG3	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
1:C:226:LEU:O	1:C:227:ASP:HB2	1.93	0.68
1:C:27:VAL:HG12	1:C:29:ILE:HG13	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLN:NE2	1:A:204:ILE:HG12	2.16	0.60
1:A:96:THR:HG23	1:A:98:LEU:H	1.66	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:CB	1:B:44:ARG:HH11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:158:ARG:HD2	2:F:244:HOH:O	2.14	0.47
1:F:106:LEU:HD11	1:F:169:LEU:HD22	1.96	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:O	1:C:211:LEU:HD12	2.14	0.47
1:E:78:GLY:HA2	1:E:85:THR:HB	1.96	0.46
1:A:79:GLY:N	1:A:85:THR:HG22	2.19	0.46
1:A:25:GLN:HG2	1:A:25:GLN:H	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:213:LEU:HD12	1:B:213:LEU:C	2.37	0.45
1:D:140:VAL:HG22	1:D:163:GLN:HG3	1.99	0.45
1:D:96:THR:CG2	1:D:98:LEU:H	2.30	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: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:169:LEU:C	1:D:169:LEU:HD12	2.38	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
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:HD2	1:E:73:ARG:HH11	1.55	0.44
1:F:221:ILE:HG13	1:F:221:ILE:H	1.60	0.43
1:B:169:LEU:HD12	1:B:169:LEU:C	2.38	0.43
1:D:211:LEU:H	1:D:211:LEU:HD23	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: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:226:LEU:O	1:C:227:ASP:CB	2.62	0.43
1:C:96:THR:CG2	1:C:98:LEU:H	2.32	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:C:12:ALA:HB3	1:C:85:THR:HG21	2.02	0.42
1:E:211:LEU:O	1:E:211:LEU:HD12	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:NH2	1:E:158:ARG:CG	2.80	0.42
1:F:143:THR:HG21	1:F:145:LYS:HZ3	1.84	0.42
1:B:169:LEU:C	1:B:169:LEU:CD1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:VAL:CG2	1:F:76:LYS:HG2	2.50	0.42
1:C:146:ARG:HD2	1:C:146:ARG:HH21	1.64	0.42
1:C:211:LEU:C	1:C:211:LEU:HD12	2.40	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:C:169:LEU:C	1:C:169:LEU:HD12	2.41	0.41
1:E:106:LEU:HD11	1:E:169:LEU:HD22	2.03	0.41
1:E:33:THR:HG21	1:E:61:PHE:CE2	2.55	0.41
1:B:126:GLN:HE21	1:B:204:ILE:HG12	1.86	0.41
1:E:146:ARG:HH11	1:E:146:ARG:HG3	1.86	0.41
1:A:5:ASN:OD1	1:A:104:ASN:HB2	2.19	0.41
1:A:2:LYS:HG2	1:D:200:ARG:NH2	2.35	0.41
1:A:75:TRP:HB3	1:A:77:ASN:OD1	2.21	0.41
1:B:177:ARG:HB2	1:B:177:ARG:HE	1.66	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:NH1	1:E:146:ARG:HG3	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 [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	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 [i](#)

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%)	152 (93%)	11 (7%)	16	17
1	B	166/180 (92%)	152 (92%)	14 (8%)	11	10
1	C	165/180 (92%)	155 (94%)	10 (6%)	18	20
1	D	164/180 (91%)	150 (92%)	14 (8%)	10	10
1	E	164/180 (91%)	149 (91%)	15 (9%)	9	8
1	F	162/180 (90%)	151 (93%)	11 (7%)	16	16
All	All	984/1080 (91%)	909 (92%)	75 (8%)	13	13

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	56	SER
1	A	81	THR
1	A	85	THR

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	96	THR
1	A	138	VAL
1	A	159	SER
1	A	169	LEU
1	A	197	LEU
1	A	227	ASP
1	B	1	LEU
1	B	44	ARG
1	B	85	THR
1	B	94	LEU
1	B	96	THR
1	B	149	SER
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	56	SER
1	C	85	THR
1	C	94	LEU
1	C	96	THR
1	C	148	GLU
1	C	158	ARG
1	C	169	LEU
1	C	197	LEU
1	C	217	GLN
1	D	3	ARG
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	156	VAL
1	D	158	ARG

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Mol	Chain	Res	Type
1	D	159	SER
1	D	169	LEU
1	D	197	LEU
1	E	1	LEU
1	E	31	SER
1	E	56	SER
1	E	60	THR
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	31	SER
1	F	32	LYS
1	F	58	GLU
1	F	85	THR
1	F	94	LEU
1	F	96	THR
1	F	151	GLN
1	F	156	VAL
1	F	158	ARG
1	F	169	LEU
1	F	197	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	80	GLN
1	A	126	GLN
1	B	80	GLN
1	B	126	GLN
1	B	151	GLN
1	C	80	GLN
1	C	163	GLN
1	D	66	GLN

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Mol	Chain	Res	Type
1	D	80	GLN
1	D	163	GLN
1	D	171	GLN
1	E	80	GLN
1	E	126	GLN
1	F	25	GLN
1	F	37	HIS
1	F	80	GLN
1	F	126	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](#)

There are no ligands in this entry.

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	212/231 (91%)	0.07	6 (2%) 53 64	22, 39, 76, 88	0
1	B	214/231 (92%)	0.10	10 (4%) 31 44	22, 38, 73, 84	0
1	C	214/231 (92%)	-0.06	7 (3%) 46 59	25, 42, 71, 90	0
1	D	211/231 (91%)	0.04	7 (3%) 46 59	28, 43, 75, 84	0
1	E	213/231 (92%)	0.02	2 (0%) 84 90	23, 37, 70, 95	0
1	F	209/231 (90%)	-0.02	6 (2%) 51 62	21, 38, 68, 82	0
All	All	1273/1386 (91%)	0.02	38 (2%) 50 61	21, 39, 74, 95	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	PRO	4.5
1	B	220	TYR	4.2
1	B	31	SER	3.8
1	A	61	PHE	3.8
1	B	184	LEU	3.4
1	C	31	SER	3.3
1	B	80	GLN	3.3
1	A	187	ILE	3.2
1	A	186	GLY	3.1
1	D	220	TYR	3.0
1	B	223	ARG	3.0
1	F	60	THR	3.0
1	D	223	ARG	2.8
1	C	80	GLN	2.8
1	D	148	GLU	2.8
1	F	148	GLU	2.8
1	C	223	ARG	2.7
1	E	61	PHE	2.7
1	D	61	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	23	PRO	2.6
1	F	79	GLY	2.6
1	D	181	ALA	2.6
1	F	80	GLN	2.6
1	B	216	PRO	2.5
1	C	29	ILE	2.5
1	F	223	ARG	2.5
1	C	220	TYR	2.4
1	B	57	PRO	2.4
1	A	216	PRO	2.3
1	A	79	GLY	2.3
1	C	224	LEU	2.3
1	F	57	PRO	2.2
1	B	72	VAL	2.2
1	D	31	SER	2.2
1	B	81	THR	2.1
1	D	224	LEU	2.1
1	B	226	LEU	2.1
1	C	23	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.