



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

PDB ID : 1IV1
Title : Structure of 2C-Methyl-D-erythritol-2,4-cyclodiphosphate Synthase
Authors : Kishida, H.; Wada, T.; Unzai, S.; Kuzuyama, T.; Terada, T.; Sirouzu, M.; Yokoyama, S.; Tame, J.R.H.; Park, S.-Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-03-11
Resolution : 1.65 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

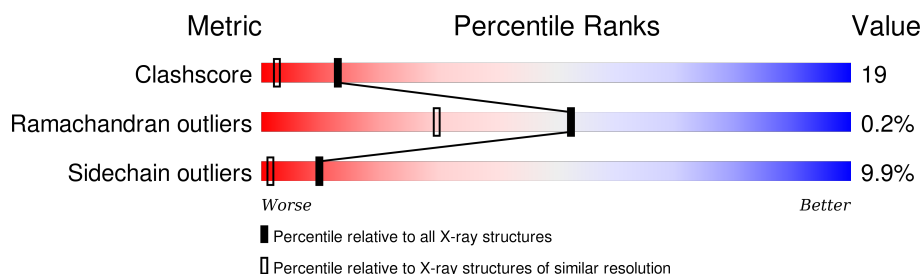
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	152	
1	B	152	
1	C	152	
1	D	152	
1	E	152	
1	F	152	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7264 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1152	729	213	209	1			
1	C	150	Total	C	N	O	S	0	0	0
			1152	729	213	209	1			
1	D	150	Total	C	N	O	S	0	0	0
			1152	729	213	209	1			
1	B	150	Total	C	N	O	S	0	0	0
			1152	729	213	209	1			
1	E	150	Total	C	N	O	S	0	0	0
			1152	729	213	209	1			
1	F	150	Total	C	N	O	S	0	0	0
			1152	729	213	209	1			

- Molecule 2 is water.

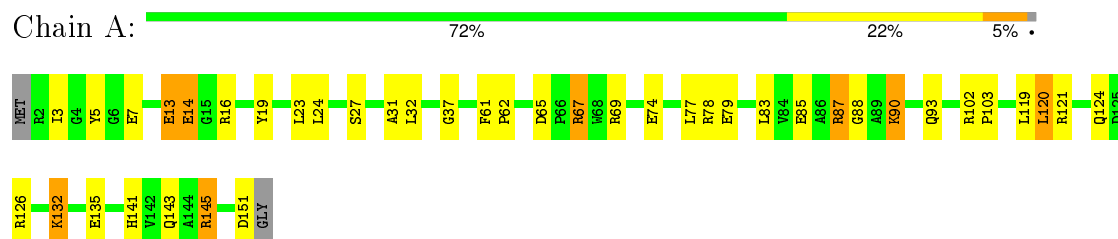
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	B	73	Total	O	0	0
			73	73		
2	C	82	Total	O	0	0
			82	82		
2	D	36	Total	O	0	0
			36	36		
2	E	31	Total	O	0	0
			31	31		
2	F	58	Total	O	0	0
			58	58		

3 Residue-property plots

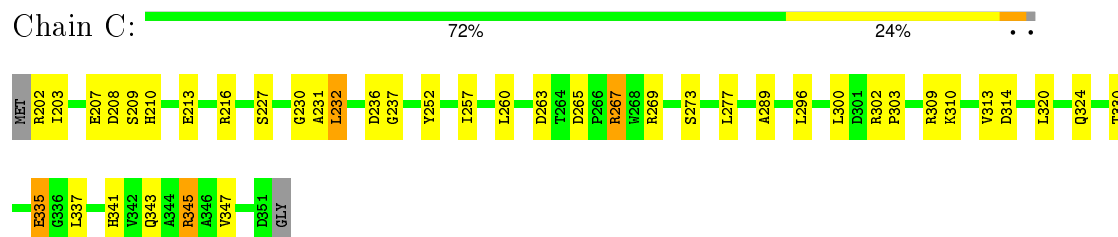
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

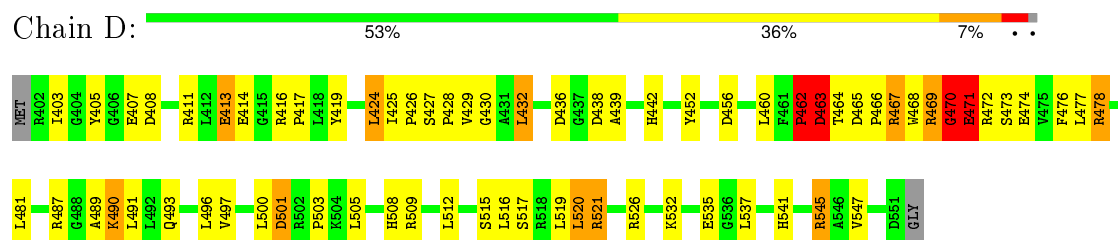
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



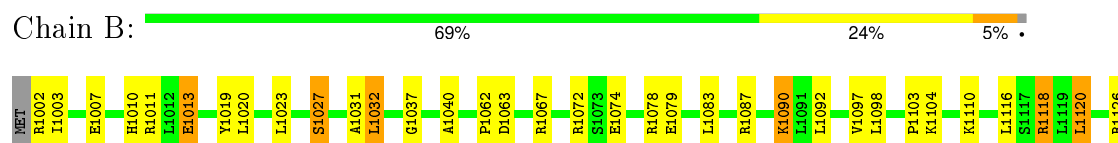
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

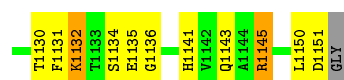


- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



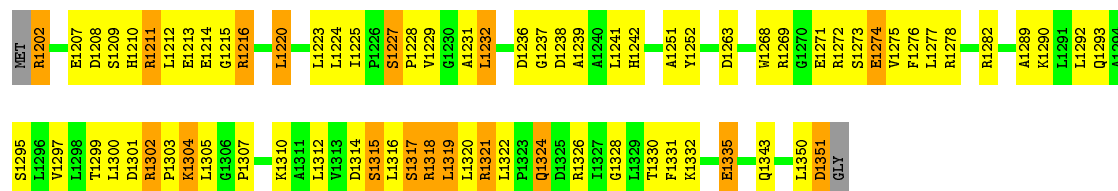
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase





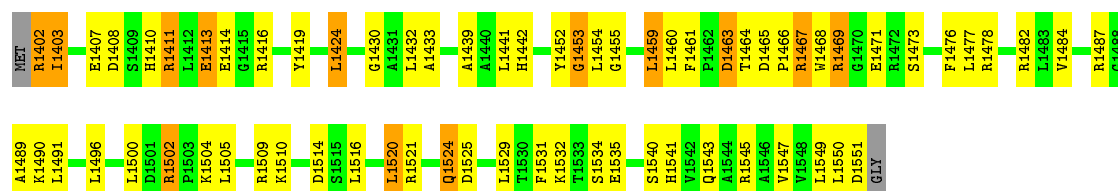
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain E: 49% 38% 11%



- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain F: 54% 36% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.83Å 105.83Å 148.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65	Depositor
% Data completeness (in resolution range)	91.3 (20.00-1.65)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.228 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7264	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.35	0/1173	1.09	3/1590 (0.2%)
1	B	0.35	0/1173	1.03	4/1590 (0.3%)
1	C	0.38	0/1173	1.09	4/1590 (0.3%)
1	D	0.48	1/1173 (0.1%)	1.11	7/1590 (0.4%)
1	E	0.32	0/1173	1.07	6/1590 (0.4%)
1	F	0.36	0/1173	1.08	4/1590 (0.3%)
All	All	0.38	1/7038 (0.0%)	1.08	28/9540 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	470	GLY	C-N	-7.61	1.16	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	463	ASP	N-CA-CB	-10.80	91.17	110.60
1	B	1145	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	526	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	E	1202	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	D	462	PRO	O-C-N	-7.45	110.78	122.70
1	D	545	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	C	267	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	A	145	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	126	ARG	NE-CZ-NH1	6.84	123.72	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1550	LEU	C-N-CA	6.73	138.52	121.70
1	C	265	ASP	CB-CG-OD1	6.50	124.15	118.30
1	E	1211	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	E	1202	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	F	1502	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	E	1318	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	1002	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	F	1502	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	309	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	D	478	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	345	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	1072	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	F	1509	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	470	GLY	C-N-CA	5.13	134.54	121.70
1	B	1150	LEU	C-N-CA	5.11	134.46	121.70
1	E	1318	ARG	CD-NE-CZ	5.09	130.73	123.60
1	A	69	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	460	LEU	CA-CB-CG	5.05	126.92	115.30
1	E	1282	ARG	CD-NE-CZ	5.02	130.63	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	462	PRO	Mainchain,Peptide
1	D	470	GLY	Mainchain,Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1152	0	1188	34	0
1	B	1152	0	1188	40	0
1	C	1152	0	1188	39	0
1	D	1152	0	1187	58	0
1	E	1152	0	1188	68	0
1	F	1152	0	1188	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	72	0	0	1	0
2	B	73	0	0	5	0
2	C	82	0	0	3	0
2	D	36	0	0	3	0
2	E	31	0	0	2	0
2	F	58	0	0	4	0
All	All	7264	0	7127	268	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 19.

All (268) 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:207:GLU:HG2	1:C:345:ARG:HG2	1.45	0.98
1:B:1007:GLU:HG2	1:B:1145:ARG:HG2	1.44	0.97
1:F:1469:ARG:HB3	1:F:1469:ARG:HH11	1.37	0.90
1:F:1459:LEU:HG	1:F:1460:LEU:HD23	1.55	0.88
1:F:1407:GLU:HG2	1:F:1545:ARG:HG2	1.59	0.85
1:A:7:GLU:HG3	1:D:497:VAL:HG21	1.59	0.84
1:E:1310:LYS:HE2	1:E:1314:ASP:OD2	1.78	0.83
1:E:1213:GLU:HB3	1:E:1216:ARG:HG3	1.62	0.81
1:E:1300:LEU:HD11	1:E:1303:PRO:HD2	1.65	0.79
1:F:1504:LYS:HD3	2:F:303:HOH:O	1.83	0.79
1:B:1143:GLN:HE21	1:B:1145:ARG:HH22	1.28	0.78
1:D:481:LEU:HD13	1:D:521:ARG:HH21	1.48	0.78
1:D:416:ARG:HB2	1:D:430:GLY:H	1.48	0.78
1:B:1090:LYS:HB2	1:B:1151:ASP:HA	1.66	0.78
1:D:427:SER:HB3	1:D:503:PRO:HG3	1.68	0.76
1:B:1092:LEU:O	1:B:1126:ARG:HD2	1.86	0.75
1:B:1007:GLU:OE2	1:F:1545:ARG:HD2	1.87	0.74
1:D:407:GLU:HG2	1:D:545:ARG:HG2	1.69	0.74
1:E:1274:GLU:O	1:E:1278:ARG:HG3	1.88	0.73
1:E:1272:ARG:HG3	2:E:141:HOH:O	1.88	0.72
1:A:65:ASP:OD1	1:A:67:ARG:HB2	1.89	0.71
1:A:132:LYS:HE3	1:C:207:GLU:O	1.91	0.71
1:A:7:GLU:OE2	1:D:545:ARG:HD2	1.90	0.70
1:E:1305:LEU:HD22	1:E:1312:LEU:HD11	1.74	0.69
1:E:1263:ASP:O	1:E:1269:ARG:HD3	1.92	0.68
1:B:1027:SER:HB2	1:B:1103:PRO:HG3	1.74	0.68
1:C:213:GLU:OE1	1:C:232:LEU:HB2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1310:LYS:HG2	1:E:1314:ASP:OD2	1.95	0.67
1:F:1453:GLY:O	1:F:1454:LEU:HD23	1.93	0.67
1:B:1143:GLN:NE2	1:B:1145:ARG:HH22	1.91	0.67
1:D:515:SER:O	1:D:519:LEU:HD13	1.94	0.67
1:D:481:LEU:HD13	1:D:521:ARG:NH2	2.08	0.67
1:E:1214:GLU:OE2	1:E:1228:PRO:HB2	1.94	0.67
1:F:1441:LEU:HD22	1:F:1477:LEU:HD22	1.76	0.66
1:A:3:ILE:H	1:D:493:GLN:NE2	1.93	0.66
1:A:27:SER:HB2	1:A:103:PRO:HG3	1.77	0.66
1:A:13:GLU:OE1	1:A:32:LEU:HD22	1.95	0.65
1:A:5:TYR:OH	1:A:145:ARG:HG2	1.97	0.65
1:B:1135:GLU:HG3	1:E:1209:SER:O	1.97	0.65
1:E:1316:LEU:O	1:E:1320:LEU:HB2	1.97	0.65
1:E:1305:LEU:HD13	1:E:1312:LEU:HD13	1.77	0.65
1:E:1220:LEU:HD13	1:E:1305:LEU:HD11	1.80	0.64
1:C:267:ARG:HG3	2:C:382:HOH:O	1.97	0.64
1:F:1543:GLN:HE21	1:F:1545:ARG:HH22	1.44	0.63
1:D:478:ARG:NH2	1:D:519:LEU:HA	2.12	0.63
1:D:452:TYR:OH	1:D:489:ALA:HB2	1.98	0.63
1:B:1136:GLY:HA3	1:E:1211:ARG:HH21	1.63	0.63
1:D:465:ASP:OD1	1:D:467:ARG:HD3	1.99	0.63
1:B:1013:GLU:OE1	1:B:1032:LEU:HD13	1.98	0.63
1:F:1543:GLN:NE2	1:F:1545:ARG:HH22	1.96	0.62
1:D:465:ASP:HB3	1:D:468:TRP:CD1	2.34	0.62
1:C:252:TYR:OH	1:C:289:ALA:HB2	2.00	0.62
1:A:88:GLY:O	1:A:90:LYS:HE2	2.00	0.62
1:F:1452:TYR:CE1	1:F:1489:ALA:HB2	2.35	0.61
1:B:1143:GLN:HE21	1:B:1145:ARG:NH2	1.97	0.61
1:F:1531:PHE:O	1:F:1532:LYS:HD2	2.00	0.61
1:E:1304:LYS:O	1:E:1307:PRO:HD2	2.01	0.61
1:B:1145:ARG:HD2	1:E:1207:GLU:OE2	2.00	0.60
1:E:1223:LEU:HD11	1:E:1315:SER:OG	2.01	0.60
1:E:1300:LEU:HD12	1:E:1302:ARG:O	2.03	0.59
1:C:252:TYR:CZ	1:C:289:ALA:HB2	2.36	0.59
1:D:419:TYR:CE1	1:D:424:LEU:HD23	2.37	0.59
1:D:413:GLU:OE1	1:D:432:LEU:HD13	2.03	0.59
1:F:1500:LEU:HD21	1:F:1505:LEU:HD11	1.85	0.59
1:F:1452:TYR:HE1	1:F:1489:ALA:HB2	1.68	0.58
1:D:470:GLY:O	1:D:471:GLU:O	2.21	0.58
1:D:414:GLU:HA	1:D:428:PRO:O	2.04	0.57
1:F:1463:ASP:O	1:F:1469:ARG:HD3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1466:PRO:HA	1:F:1469:ARG:NH2	2.19	0.57
1:E:1214:GLU:HG3	1:E:1215:GLY:N	2.19	0.57
1:F:1490:LYS:O	1:F:1490:LYS:HG3	2.03	0.57
1:E:1225:ILE:HD11	1:E:1312:LEU:HD21	1.86	0.57
1:F:1416:ARG:HH11	1:F:1416:ARG:HG2	1.69	0.56
1:A:3:ILE:H	1:D:493:GLN:HE22	1.51	0.56
1:D:452:TYR:CZ	1:D:489:ALA:HB2	2.40	0.56
1:F:1496:LEU:HD21	1:F:1529:LEU:HD13	1.87	0.56
1:B:1031:ALA:CB	1:B:1037:GLY:HA3	2.36	0.55
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.06	0.55
1:B:1011:ARG:HG3	1:B:1011:ARG:HH11	1.72	0.54
1:B:1116:LEU:O	1:B:1120:LEU:HB2	2.06	0.54
1:D:436:ASP:OD2	1:D:438:ASP:HB2	2.07	0.54
1:C:277:LEU:HD21	1:C:320:LEU:CD1	2.38	0.54
1:C:330:THR:HG22	1:D:456:ASP:HB3	1.89	0.54
1:D:508:HIS:O	1:D:512:LEU:HG	2.08	0.54
1:E:1293:GLN:HE22	1:F:1402:ARG:HG2	1.73	0.54
1:D:474:GLU:O	1:D:478:ARG:HG3	2.07	0.53
1:A:93:GLN:NE2	1:C:203:ILE:H	2.06	0.53
1:D:432:LEU:O	1:D:432:LEU:HD23	2.09	0.53
1:F:1455:GLY:HA3	1:F:1459:LEU:HD23	1.90	0.53
1:E:1231:ALA:HB1	1:E:1237:GLY:HA3	1.91	0.52
1:A:143:GLN:NE2	1:A:145:ARG:HH22	2.08	0.52
1:E:1293:GLN:HE22	1:F:1402:ARG:CG	2.22	0.52
1:C:343:GLN:NE2	1:C:345:ARG:HH22	2.08	0.51
1:E:1210:HIS:HE1	1:E:1242:HIS:ND1	2.08	0.51
1:E:1208:ASP:OD2	1:E:1242:HIS:HB2	2.10	0.51
1:A:74:GLU:O	1:A:78:ARG:HG2	2.10	0.51
1:D:473:SER:HA	1:D:476:PHE:CD2	2.45	0.51
1:F:1469:ARG:CB	1:F:1469:ARG:HH11	2.17	0.51
1:E:1213:GLU:O	1:E:1229:VAL:HA	2.11	0.51
1:A:141:HIS:HE1	1:D:535:GLU:O	1.94	0.51
1:D:509:ARG:HD3	2:D:94:HOH:O	2.10	0.51
1:B:1141:HIS:HE1	1:F:1535:GLU:O	1.94	0.50
1:D:501:ASP:HB3	2:D:112:HOH:O	2.11	0.50
1:E:1227:SER:OG	1:E:1303:PRO:HD3	2.12	0.50
1:B:1090:LYS:CB	1:B:1151:ASP:HA	2.39	0.50
1:F:1482:ARG:HD2	2:F:251:HOH:O	2.11	0.50
1:A:135:GLU:O	1:C:341:HIS:HE1	1.94	0.50
1:E:1305:LEU:HD12	1:E:1331:PHE:CD1	2.47	0.50
1:F:1414:GLU:N	1:F:1414:GLU:OE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD21	1:A:120:LEU:CD1	2.41	0.50
1:A:124:GLN:HB3	2:A:211:HOH:O	2.10	0.50
1:E:1220:LEU:CD1	1:E:1305:LEU:HD11	2.40	0.50
1:D:463:ASP:O	1:D:465:ASP:O	2.30	0.50
1:D:417:PRO:HB2	1:D:419:TYR:CE2	2.47	0.49
1:E:1202:ARG:HD3	1:E:1251:ALA:O	2.12	0.49
1:A:31:ALA:CB	1:A:37:GLY:HA3	2.42	0.49
1:C:267:ARG:NH1	2:C:428:HOH:O	2.43	0.49
1:F:1500:LEU:HD21	1:F:1505:LEU:CD1	2.43	0.49
1:D:405:TYR:HD1	1:D:547:VAL:HG22	1.77	0.49
1:F:1411:ARG:NH1	1:F:1540:SER:OG	2.46	0.49
1:E:1216:ARG:HH11	1:E:1216:ARG:HG2	1.76	0.49
1:E:1208:ASP:OD2	1:E:1239:ALA:HA	2.13	0.49
1:E:1350:LEU:O	1:E:1351:ASP:O	2.30	0.49
1:D:413:GLU:O	1:D:429:VAL:HA	2.12	0.48
1:D:452:TYR:CE1	1:D:489:ALA:HB2	2.48	0.48
1:E:1216:ARG:HE	1:E:1232:LEU:HD12	1.78	0.48
1:D:419:TYR:CZ	1:D:424:LEU:HD23	2.48	0.48
1:B:1003:ILE:HD13	1:F:1547:VAL:HG11	1.95	0.48
1:E:1236:ASP:OD2	1:E:1273:SER:OG	2.30	0.48
1:E:1335:GLU:O	1:F:1541:HIS:HE1	1.96	0.48
1:E:1213:GLU:OE1	1:E:1232:LEU:HD13	2.13	0.48
1:B:1136:GLY:HA3	1:E:1211:ARG:NH2	2.27	0.48
1:E:1293:GLN:HB2	1:E:1326:ARG:HH11	1.79	0.48
1:C:335:GLU:O	1:D:541:HIS:HE1	1.97	0.48
1:E:1305:LEU:HD13	1:E:1312:LEU:CD1	2.42	0.48
1:D:491:LEU:HD21	1:D:520:LEU:HG	1.96	0.47
1:E:1302:ARG:O	1:E:1302:ARG:HG2	2.07	0.47
1:C:267:ARG:HG2	1:B:1087:ARG:NH2	2.30	0.47
1:A:135:GLU:OE1	1:C:210:HIS:ND1	2.47	0.47
1:E:1297:VAL:HG22	1:E:1330:THR:OG1	2.15	0.47
1:B:1097:VAL:HG22	1:B:1130:THR:OG1	2.15	0.47
1:B:1019:TYR:HA	1:B:1023:LEU:O	2.14	0.47
1:F:1516:LEU:O	1:F:1520:LEU:HB2	2.14	0.47
1:B:1132:LYS:HE3	2:B:179:HOH:O	2.14	0.47
1:F:1491:LEU:CD2	1:F:1520:LEU:HG	2.45	0.47
1:E:1317:SER:OG	1:E:1322:LEU:O	2.25	0.47
1:F:1465:ASP:OD1	1:F:1467:ARG:NE	2.48	0.47
1:B:1020:LEU:HD21	2:B:352:HOH:O	2.14	0.47
1:C:252:TYR:CE1	1:C:289:ALA:HB2	2.50	0.47
1:B:1031:ALA:HB1	1:B:1037:GLY:HA3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1478:ARG:HH11	1:F:1478:ARG:HG2	1.80	0.46
1:F:1484:VAL:O	1:F:1487:ARG:HB2	2.15	0.46
1:E:1293:GLN:NE2	1:F:1403:ILE:H	2.14	0.46
1:B:1132:LYS:HD2	1:B:1132:LYS:HA	1.62	0.46
1:E:1263:ASP:HB2	1:E:1269:ARG:HG3	1.98	0.46
1:A:74:GLU:OE2	1:A:78:ARG:NH2	2.49	0.46
1:B:1074:GLU:OE2	1:B:1078:ARG:NE	2.49	0.46
1:F:1491:LEU:HD21	1:F:1520:LEU:HG	1.97	0.46
1:E:1231:ALA:CB	1:E:1237:GLY:HA3	2.46	0.46
1:C:296:LEU:N	1:C:296:LEU:HD23	2.31	0.46
1:E:1212:LEU:HD13	1:E:1229:VAL:HG21	1.98	0.46
1:D:467:ARG:O	1:D:467:ARG:HG2	2.16	0.45
1:C:208:ASP:OD2	1:C:210:HIS:NE2	2.49	0.45
1:F:1464:THR:O	1:F:1469:ARG:NH2	2.49	0.45
1:B:1131:PHE:O	1:B:1132:LYS:HD2	2.16	0.45
1:D:413:GLU:HB3	1:D:416:ARG:HG3	1.98	0.45
1:A:143:GLN:HE21	1:A:145:ARG:HH22	1.64	0.45
1:D:462:PRO:O	1:D:464:THR:N	2.49	0.45
1:F:1463:ASP:N	1:F:1463:ASP:OD1	2.50	0.45
1:E:1252:TYR:CE1	1:E:1289:ALA:HB2	2.51	0.45
1:E:1301:ASP:OD1	1:E:1301:ASP:N	2.50	0.45
1:D:408:ASP:OD2	1:D:442:HIS:HB2	2.16	0.45
1:F:1432:LEU:O	1:F:1433:ALA:HB2	2.16	0.45
1:C:313:VAL:HG12	1:C:324:GLN:NE2	2.32	0.45
1:F:1487:ARG:HH11	1:F:1487:ARG:HG2	1.81	0.45
1:C:269:ARG:HB3	1:C:269:ARG:HH11	1.81	0.45
1:A:19:TYR:HA	1:A:23:LEU:O	2.16	0.45
1:C:232:LEU:HA	2:C:425:HOH:O	2.18	0.44
1:D:500:LEU:HD21	1:D:505:LEU:CD1	2.46	0.44
1:E:1278:ARG:NH1	2:E:187:HOH:O	2.50	0.44
1:C:213:GLU:OE2	1:C:232:LEU:HD13	2.17	0.44
1:E:1271:GLU:HB3	1:E:1275:VAL:HG21	1.98	0.44
1:C:227:SER:HB2	1:C:303:PRO:HG3	1.99	0.44
1:B:1062:PRO:HA	2:B:287:HOH:O	2.18	0.44
1:E:1299:THR:HB	1:E:1343:GLN:HB2	2.00	0.44
1:E:1238:ASP:OD1	1:E:1241:LEU:HG	2.17	0.44
1:D:472:ARG:NH1	2:D:96:HOH:O	2.49	0.44
1:D:427:SER:HB3	1:D:503:PRO:CG	2.44	0.44
1:D:477:LEU:HD21	1:D:520:LEU:HD13	1.99	0.44
1:F:1461:PHE:CE2	1:F:1476:PHE:HB3	2.52	0.44
1:F:1534:SER:O	1:F:1535:GLU:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:ILE:CD1	1:F:1547:VAL:HG11	2.48	0.44
1:D:425:ILE:HA	1:D:426:PRO:HD3	1.84	0.44
1:F:1410:HIS:HE1	1:F:1439:ALA:HA	1.83	0.44
1:F:1465:ASP:O	1:F:1469:ARG:NH1	2.50	0.44
1:F:1465:ASP:C	1:F:1469:ARG:HH12	2.20	0.44
1:E:1320:LEU:O	1:E:1321:ARG:NE	2.51	0.44
1:C:314:ASP:OD1	1:C:324:GLN:NE2	2.50	0.44
1:E:1216:ARG:HD2	1:E:1232:LEU:HB2	1.99	0.44
1:A:16:ARG:NH1	1:A:31:ALA:O	2.51	0.44
1:E:1317:SER:OG	1:E:1324:GLN:NE2	2.38	0.43
1:F:1487:ARG:HD3	1:F:1487:ARG:HA	1.82	0.43
1:C:310:LYS:NZ	1:C:314:ASP:OD2	2.51	0.43
1:B:1010:HIS:HD2	1:F:1535:GLU:OE2	2.02	0.43
1:B:1027:SER:HB2	1:B:1103:PRO:CG	2.45	0.43
1:C:202:ARG:HD2	1:C:252:TYR:CE1	2.53	0.43
1:E:1295:SER:HA	1:E:1328:GLY:O	2.19	0.43
1:D:496:LEU:H	1:D:496:LEU:HD23	1.83	0.43
1:A:7:GLU:HG3	1:D:497:VAL:CG2	2.40	0.43
1:F:1461:PHE:CD2	1:F:1476:PHE:HB3	2.54	0.43
1:D:490:LYS:HB2	1:D:490:LYS:HE3	1.74	0.43
1:E:1277:LEU:HD21	1:E:1320:LEU:CD1	2.49	0.43
1:C:216:ARG:O	1:C:230:GLY:HA3	2.18	0.43
1:B:1079:GLU:O	1:B:1083:LEU:HG	2.19	0.43
1:B:1141:HIS:HD2	2:B:146:HOH:O	2.02	0.42
1:E:1351:ASP:N	1:E:1351:ASP:OD1	2.52	0.42
1:D:496:LEU:N	1:D:496:LEU:HD23	2.34	0.42
1:A:74:GLU:OE2	1:A:119:LEU:HG	2.18	0.42
1:C:257:ILE:HG21	1:C:257:ILE:HD13	1.88	0.42
1:B:1097:VAL:HG21	1:E:1207:GLU:HG3	2.01	0.42
1:A:67:ARG:HH11	1:A:67:ARG:HG2	1.83	0.42
1:F:1514:ASP:HA	1:F:1524:GLN:HE22	1.84	0.42
1:F:1465:ASP:HB3	1:F:1468:TRP:HD1	1.84	0.42
1:F:1419:TYR:CE1	1:F:1424:LEU:HG	2.54	0.42
1:B:1040:ALA:HB2	1:B:1098:LEU:HD21	2.01	0.42
1:E:1331:PHE:O	1:E:1332:LYS:HD2	2.19	0.42
1:D:516:LEU:O	1:D:520:LEU:HB2	2.19	0.42
1:E:1216:ARG:NH1	1:E:1216:ARG:HG2	2.33	0.42
1:C:260:LEU:HD22	1:B:1067:ARG:HH21	1.85	0.42
1:F:1478:ARG:HG2	1:F:1478:ARG:NH1	2.34	0.42
1:C:202:ARG:HD2	1:C:252:TYR:CZ	2.54	0.42
1:F:1452:TYR:CE2	1:F:1487:ARG:HB3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LEU:HD22	1:B:1067:ARG:NH2	2.35	0.42
1:B:1104:LYS:HD2	1:B:1104:LYS:HA	1.85	0.42
1:A:83:LEU:O	1:A:87:ARG:HD2	2.19	0.42
1:C:236:ASP:OD2	1:C:273:SER:OG	2.37	0.41
1:F:1413:GLU:N	1:F:1430:GLY:O	2.50	0.41
1:C:337:LEU:HD12	1:C:337:LEU:O	2.20	0.41
1:A:61:PHE:N	1:A:62:PRO:HD3	2.36	0.41
1:E:1319:LEU:HD12	1:E:1319:LEU:HA	1.90	0.41
1:E:1211:ARG:NH1	1:E:1211:ARG:HG3	2.35	0.41
1:E:1293:GLN:NE2	1:E:1326:ARG:HH11	2.18	0.41
1:C:231:ALA:HB3	1:C:237:GLY:HA3	2.02	0.41
1:C:347:VAL:HG11	1:D:403:ILE:CD1	2.51	0.41
1:C:213:GLU:OE1	1:C:232:LEU:HD13	2.20	0.41
1:F:1549:LEU:HG	2:F:289:HOH:O	2.20	0.41
1:F:1473:SER:HB3	2:F:118:HOH:O	2.20	0.41
1:F:1468:TRP:O	1:F:1471:GLU:HG2	2.20	0.41
1:C:296:LEU:HD23	1:C:296:LEU:H	1.85	0.41
1:D:408:ASP:OD2	1:D:439:ALA:HA	2.21	0.41
1:A:102:ARG:HB2	1:A:103:PRO:HA	2.03	0.41
1:D:478:ARG:HH22	1:D:519:LEU:HA	1.82	0.41
1:F:1487:ARG:NH1	1:F:1487:ARG:HG2	2.36	0.41
1:D:532:LYS:HB3	1:D:532:LYS:HE3	1.84	0.41
1:D:537:LEU:HD12	1:D:537:LEU:HA	1.88	0.41
1:B:1118:ARG:HD3	2:B:328:HOH:O	2.20	0.41
1:D:466:PRO:HA	1:D:469:ARG:HH21	1.86	0.41
1:C:267:ARG:NH1	1:C:267:ARG:HB2	2.36	0.40
1:A:85:GLU:OE2	1:A:121:ARG:NH2	2.49	0.40
1:D:481:LEU:HA	1:D:481:LEU:HD23	1.93	0.40
1:F:1408:ASP:OD2	1:F:1442:HIS:ND1	2.55	0.40
1:A:14:GLU:OE1	1:A:102:ARG:NH2	2.50	0.40
1:E:1229:VAL:HG21	1:E:1302:ARG:HD3	2.03	0.40
1:E:1268:TRP:HB3	1:E:1276:PHE:CE1	2.57	0.40
1:D:413:GLU:O	1:D:416:ARG:HB2	2.21	0.40
1:A:3:ILE:HD11	1:C:203:ILE:CD1	2.52	0.40
1:E:1293:GLN:NE2	1:E:1326:ARG:NH1	2.69	0.40
1:A:19:TYR:CE1	1:A:24:LEU:HD23	2.56	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	148/152 (97%)	146 (99%)	2 (1%)	0	100	100
1	B	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
1	C	148/152 (97%)	146 (99%)	2 (1%)	0	100	100
1	D	148/152 (97%)	139 (94%)	8 (5%)	1 (1%)	26	7
1	E	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
1	F	148/152 (97%)	139 (94%)	8 (5%)	1 (1%)	26	7
All	All	888/912 (97%)	855 (96%)	31 (4%)	2 (0%)	52	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	471	GLU
1	F	1453	GLY

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	121/122 (99%)	113 (93%)	8 (7%)	21	4
1	B	121/122 (99%)	111 (92%)	10 (8%)	14	2
1	C	121/122 (99%)	115 (95%)	6 (5%)	30	7
1	D	121/122 (99%)	107 (88%)	14 (12%)	7	1
1	E	121/122 (99%)	103 (85%)	18 (15%)	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	121/122 (99%)	105 (87%)	16 (13%)	5	0
All	All	726/732 (99%)	654 (90%)	72 (10%)	10	1

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

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	67	ARG
1	A	87	ARG
1	A	90	LYS
1	A	120	LEU
1	A	132	LYS
1	A	151	ASP
1	C	209	SER
1	C	232	LEU
1	C	263	ASP
1	C	300	LEU
1	C	302	ARG
1	C	335	GLU
1	D	411	ARG
1	D	413	GLU
1	D	424	LEU
1	D	432	LEU
1	D	463	ASP
1	D	467	ARG
1	D	469	ARG
1	D	471	GLU
1	D	487	ARG
1	D	490	LYS
1	D	501	ASP
1	D	517	SER
1	D	520	LEU
1	D	521	ARG
1	B	1013	GLU
1	B	1027	SER
1	B	1032	LEU
1	B	1063	ASP
1	B	1090	LYS
1	B	1110	LYS
1	B	1118	ARG
1	B	1120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1132	LYS
1	B	1134	SER
1	E	1216	ARG
1	E	1220	LEU
1	E	1224	LEU
1	E	1227	SER
1	E	1232	LEU
1	E	1274	GLU
1	E	1290	LYS
1	E	1292	LEU
1	E	1302	ARG
1	E	1304	LYS
1	E	1315	SER
1	E	1317	SER
1	E	1318	ARG
1	E	1319	LEU
1	E	1321	ARG
1	E	1324	GLN
1	E	1335	GLU
1	E	1351	ASP
1	F	1402	ARG
1	F	1403	ILE
1	F	1411	ARG
1	F	1413	GLU
1	F	1424	LEU
1	F	1459	LEU
1	F	1463	ASP
1	F	1467	ARG
1	F	1469	ARG
1	F	1502	ARG
1	F	1510	LYS
1	F	1520	LEU
1	F	1521	ARG
1	F	1524	GLN
1	F	1525	ASP
1	F	1551	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	93	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	141	HIS
1	A	143	GLN
1	C	293	GLN
1	C	324	GLN
1	C	341	HIS
1	C	343	GLN
1	D	410	HIS
1	D	493	GLN
1	D	541	HIS
1	B	1010	HIS
1	B	1093	GLN
1	B	1141	HIS
1	B	1143	GLN
1	E	1210	HIS
1	E	1293	GLN
1	E	1341	HIS
1	F	1493	GLN
1	F	1508	HIS
1	F	1524	GLN
1	F	1541	HIS
1	F	1543	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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.