



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:23 AM UTC

PDB ID : 3OKR / pdb_00003okr
Title : Structure of Mtb apo 2-C-methyl-D-erythritol 4-phosphate cytidyltransferase (IspD)
Authors : Sacchettini, J.C.; Reddy, M.C.M.; Bruning, J.B.; Thurman, C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2010-08-25
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
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

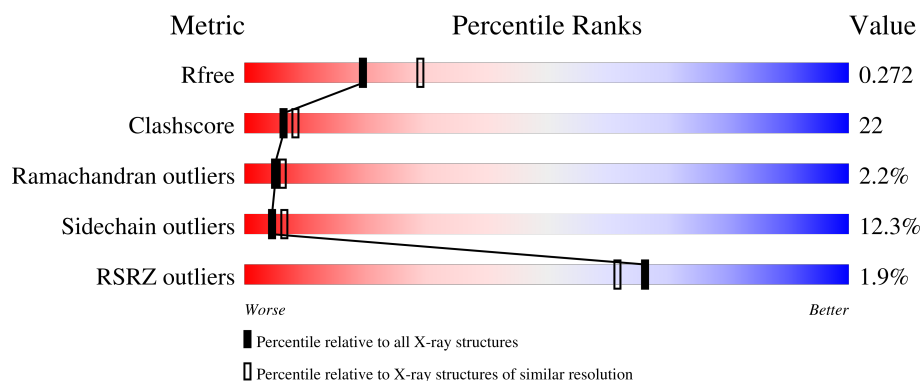
1 Overall quality at a glance

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	231	% 56% 27% 5% 12%
1	B	231	3% 58% 28% • 10%
1	C	231	2% 50% 27% 6% 16%
1	D	231	58% 27% • • 11%
2	F	7	71% 29%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5771 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 4-phosphate cytidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1439	913	250	275	1			
1	B	208	Total	C	N	O	S	0	0	0
			1469	930	254	284	1			
1	C	194	Total	C	N	O		0	0	0
			1348	857	228	263				
1	D	205	Total	C	N	O	S	0	0	0
			1434	909	246	278	1			

- Molecule 2 is a protein called Heptamer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	7	Total	C	N	O	0	0	0
			35	21	7	7			

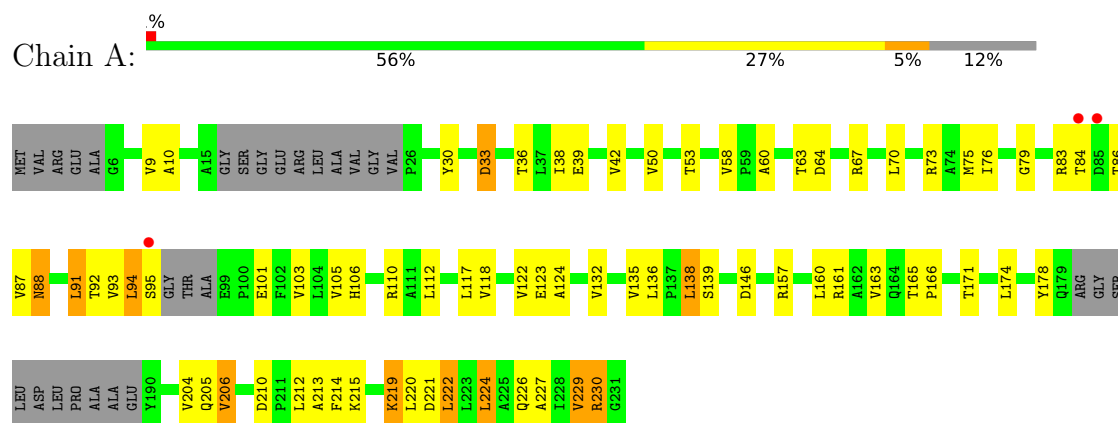
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	14	Total	O	0	0
			14	14		
3	C	10	Total	O	0	0
			10	10		
3	D	15	Total	O	0	0
			15	15		

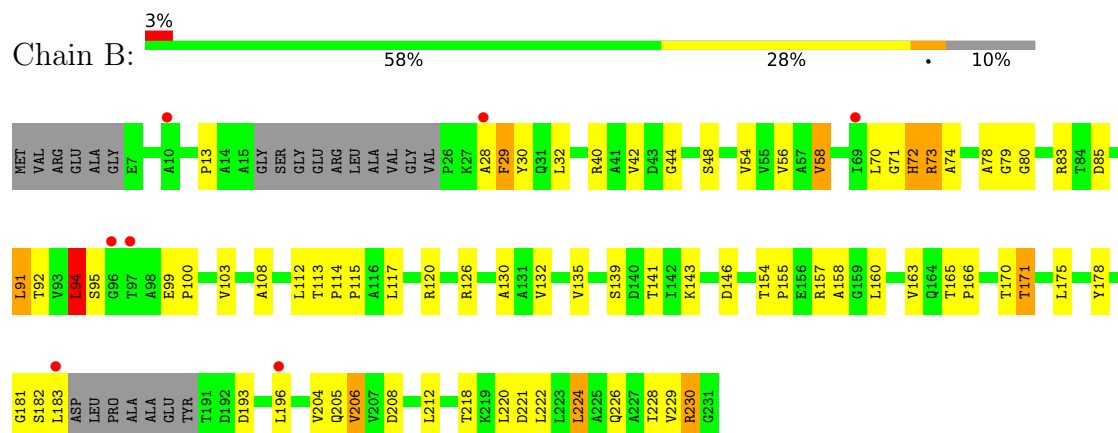
3 Residue-property plots

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

• Molecule 1: 2-C-methyl-D-erythritol 4-phosphate cytidylyltransferase

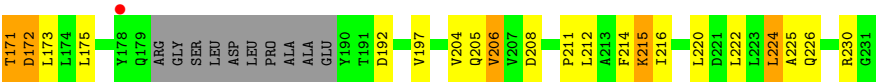


• Molecule 1: 2-C-methyl-D-erythritol 4-phosphate cytidylyltransferase

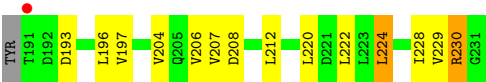


• Molecule 1: 2-C-methyl-D-erythritol 4-phosphate cytidylyltransferase

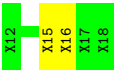




● Molecule 1: 2-C-methyl-D-erythritol 4-phosphate cytidylyltransferase



● Molecule 2: Heptamer peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.08Å 60.27Å 74.51Å 104.18° 110.52° 88.68°	Depositor
Resolution (Å)	25.05 – 2.40 25.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.9 (25.05-2.40) 95.9 (25.05-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.210 , 0.278 0.206 , 0.272	Depositor DCC
R_{free} test set	1661 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5771	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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

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	0.57	0/1456	0.91	2/1993 (0.1%)
1	B	0.62	0/1487	0.94	2/2037 (0.1%)
1	C	0.54	0/1362	0.92	0/1870
1	D	0.65	1/1451 (0.1%)	0.95	3/1989 (0.2%)
All	All	0.60	1/5756 (0.0%)	0.93	7/7889 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	93	VAL	CA-CB	8.01	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	VAL	N-CA-C	-7.61	98.62	109.51
1	D	73	ARG	N-CA-C	-6.54	105.28	113.20
1	A	210	ASP	CA-C-N	6.46	126.15	119.56
1	A	210	ASP	C-N-CA	6.46	126.15	119.56
1	B	95	SER	CB-CA-C	-6.09	107.82	116.34
1	B	158	ALA	N-CA-C	-5.47	102.79	110.50
1	D	90	ALA	N-CA-C	-5.06	105.76	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	94	LEU	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	1439	0	1427	55	0
1	B	1469	0	1458	64	0
1	C	1348	0	1313	79	0
1	D	1434	0	1413	56	0
2	F	35	0	10	3	0
3	A	7	0	0	0	0
3	B	14	0	0	1	0
3	C	10	0	0	0	0
3	D	15	0	0	0	0
All	All	5771	0	5621	248	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 22.

All (248) 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:94:LEU:HB3	1:C:95:SER:CA	1.77	1.13
1:C:94:LEU:CB	1:C:95:SER:HA	1.91	1.00
1:B:103:VAL:HG23	1:B:171:THR:HB	1.44	0.97
1:C:94:LEU:HB3	1:C:95:SER:HA	0.96	0.95
1:B:72:HIS:HA	1:B:74:ALA:N	1.80	0.95
1:B:182:SER:HA	1:B:183:LEU:C	1.90	0.95
1:C:60:ALA:N	1:C:61:ASP:HB3	1.81	0.95
1:B:72:HIS:HA	1:B:74:ALA:H	1.32	0.94
1:C:60:ALA:H	1:C:62:ARG:H	1.11	0.92
1:A:219:LYS:H	1:A:219:LYS:HD2	1.39	0.84
1:C:60:ALA:H	1:C:62:ARG:N	1.74	0.83
1:A:135:VAL:CG2	1:A:161:ARG:HB3	2.08	0.82
1:C:156:GLU:HA	1:C:158:ALA:N	1.95	0.80
1:C:60:ALA:N	1:C:62:ARG:H	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG22	1:A:166:PRO:HG3	1.65	0.79
1:D:93:VAL:O	1:D:94:LEU:HB3	1.83	0.78
1:B:103:VAL:CG2	1:B:171:THR:HB	2.13	0.78
1:B:30:TYR:HE1	1:B:222:LEU:HD21	1.51	0.76
1:B:230:ARG:O	1:B:230:ARG:HG2	1.84	0.75
1:C:106:HIS:HB2	1:C:166:PRO:HB3	1.69	0.74
1:C:93:VAL:O	1:C:94:LEU:HD13	1.87	0.74
1:D:193:ASP:HA	1:D:196:LEU:HD13	1.69	0.73
1:D:75:MET:C	1:D:76:ILE:HD12	2.13	0.73
1:A:135:VAL:HG21	1:A:161:ARG:HB3	1.70	0.72
1:A:174:LEU:HD11	1:A:178:TYR:HE2	1.55	0.71
1:C:100:PRO:HG2	1:C:171:THR:HG21	1.72	0.70
1:C:141:THR:O	1:D:163:VAL:HG12	1.92	0.70
1:A:226:GLN:O	1:A:230:ARG:HD2	1.92	0.69
1:A:135:VAL:HG22	1:A:161:ARG:HB3	1.74	0.69
1:C:88:ASN:H	1:C:88:ASN:HD22	1.38	0.69
1:C:138:LEU:HD13	1:C:142:ILE:HG13	1.76	0.68
1:B:48:SER:HA	1:B:115:PRO:HB3	1.74	0.68
1:A:87:VAL:O	1:A:91:LEU:HB2	1.94	0.67
1:C:88:ASN:H	1:C:88:ASN:ND2	1.93	0.66
1:B:193:ASP:HA	1:B:196:LEU:HD13	1.78	0.66
1:A:103:VAL:HG23	1:A:171:THR:HG22	1.76	0.66
1:C:60:ALA:H	1:C:61:ASP:HB3	1.60	0.66
1:B:100:PRO:O	1:B:171:THR:HG21	1.95	0.65
1:D:76:ILE:N	2:F:15:UNK:O	2.29	0.65
1:B:120:ARG:HH11	1:B:208:ASP:HB2	1.60	0.65
1:B:120:ARG:NH1	1:B:208:ASP:HB2	2.12	0.65
1:A:101:GLU:O	1:A:171:THR:HG23	1.95	0.64
1:C:165:THR:HB	1:C:166:PRO:HA	1.79	0.64
1:B:205:GLN:HG3	1:B:206:VAL:N	2.12	0.64
1:C:65:GLU:O	1:C:69:ILE:HG13	1.98	0.64
1:A:67:ARG:HG3	1:A:76:ILE:HD13	1.79	0.64
1:B:205:GLN:HG3	1:B:206:VAL:H	1.62	0.64
1:D:165:THR:HB	1:D:166:PRO:HA	1.78	0.63
1:C:125:LEU:HD23	1:C:129:TYR:O	1.98	0.62
1:D:224:LEU:HD22	1:D:228:ILE:CD1	2.29	0.62
1:C:138:LEU:HD13	1:C:142:ILE:CG1	2.29	0.62
1:C:156:GLU:HA	1:C:158:ALA:O	2.00	0.62
1:C:171:THR:O	1:C:175:LEU:HG	2.00	0.62
1:B:58:VAL:O	1:B:78:ALA:HA	2.01	0.61
1:C:60:ALA:CA	1:C:61:ASP:HB3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HG21	1:D:143:LYS:HD2	1.81	0.61
1:A:9:VAL:HG22	1:A:53:THR:HB	1.82	0.60
1:C:222:LEU:O	1:C:226:GLN:HG3	2.02	0.60
1:C:30:TYR:O	1:C:36:THR:HA	2.01	0.60
1:A:174:LEU:CD1	1:A:178:TYR:HE2	2.14	0.60
1:A:138:LEU:HD12	1:A:138:LEU:H	1.67	0.60
1:D:14:ALA:HB2	1:D:58:VAL:HG12	1.84	0.60
1:C:31:GLN:HA	1:C:36:THR:HA	1.84	0.59
1:C:173:LEU:HD12	1:C:173:LEU:O	2.02	0.59
1:A:135:VAL:HG12	1:A:206:VAL:HG13	1.84	0.59
1:A:106:HIS:HD2	1:A:165:THR:OG1	1.86	0.59
1:C:35:GLN:HE21	1:C:39:GLU:HG2	1.68	0.58
1:C:141:THR:HB	1:D:163:VAL:CG1	2.33	0.58
1:B:91:LEU:HG	1:B:175:LEU:HD23	1.84	0.58
1:D:100:PRO:O	1:D:171:THR:HG21	2.02	0.58
1:A:117:LEU:C	1:A:117:LEU:HD23	2.29	0.58
1:A:219:LYS:H	1:A:219:LYS:CD	2.11	0.58
1:B:226:GLN:O	1:B:230:ARG:HD2	2.04	0.58
1:D:120:ARG:NH1	1:D:208:ASP:O	2.38	0.57
1:D:138:LEU:HD13	1:D:142:ILE:CG1	2.34	0.57
1:D:130:ALA:HB1	1:D:173:LEU:HD22	1.87	0.57
1:B:182:SER:CA	1:B:183:LEU:C	2.74	0.57
1:B:58:VAL:HG22	1:B:78:ALA:HB2	1.86	0.57
1:C:60:ALA:HB3	1:C:61:ASP:CB	2.35	0.57
1:D:58:VAL:O	1:D:78:ALA:HA	2.05	0.57
1:A:101:GLU:C	1:A:171:THR:HG23	2.30	0.56
1:A:60:ALA:O	1:A:63:THR:HG22	2.05	0.56
1:C:117:LEU:O	1:C:117:LEU:HD23	2.05	0.56
1:A:38:ILE:O	1:A:42:VAL:HG23	2.04	0.56
1:D:138:LEU:HD13	1:D:142:ILE:HG13	1.88	0.56
1:B:181:GLY:HA2	1:B:183:LEU:C	2.30	0.56
1:B:120:ARG:NH1	1:B:208:ASP:O	2.38	0.56
1:D:169:PHE:CD1	1:D:197:VAL:HG21	2.41	0.56
1:C:60:ALA:N	1:C:61:ASP:CB	2.65	0.56
1:B:42:VAL:HG22	1:B:54:VAL:HG11	1.86	0.55
1:B:100:PRO:O	1:B:171:THR:CG2	2.55	0.55
1:D:169:PHE:CE1	1:D:197:VAL:HG21	2.41	0.55
1:A:94:LEU:N	1:A:95:SER:HA	2.20	0.55
1:D:31:GLN:HA	1:D:36:THR:HA	1.88	0.55
1:A:110:ARG:HG2	1:A:213:ALA:O	2.08	0.54
1:A:50:VAL:HG23	1:A:122:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:N	1:B:196:LEU:HD12	2.23	0.54
1:C:60:ALA:H	1:C:61:ASP:CB	2.20	0.54
1:C:133:VAL:HG12	1:C:167:GLN:HG2	1.90	0.54
1:B:224:LEU:O	1:B:228:ILE:HG13	2.08	0.54
1:C:163:VAL:HG21	1:D:143:LYS:CD	2.39	0.53
1:B:178:TYR:CE2	1:B:196:LEU:HD22	2.43	0.53
1:C:94:LEU:HG	1:C:95:SER:O	2.08	0.53
1:C:156:GLU:HA	1:C:157:ARG:C	2.33	0.53
1:B:141:THR:HA	1:B:157:ARG:HD2	1.91	0.52
1:D:224:LEU:HD22	1:D:228:ILE:HD11	1.90	0.52
1:D:117:LEU:CD2	1:D:166:PRO:HD2	2.40	0.52
1:C:60:ALA:HB3	1:C:61:ASP:HB3	1.91	0.52
1:B:28:ALA:O	1:B:29:PHE:HB2	2.10	0.52
1:B:80:GLY:HA3	1:B:85:ASP:HB3	1.91	0.52
1:D:93:VAL:O	1:D:94:LEU:CB	2.52	0.52
1:A:117:LEU:HD23	1:A:117:LEU:O	2.10	0.52
1:C:135:VAL:HG22	1:C:161:ARG:HB3	1.93	0.52
1:B:218:THR:O	1:B:221:ASP:HB2	2.10	0.51
1:B:230:ARG:O	1:B:230:ARG:CG	2.55	0.51
1:D:224:LEU:HD22	1:D:228:ILE:HD12	1.93	0.51
1:B:30:TYR:CE1	1:B:222:LEU:HD21	2.39	0.51
1:C:226:GLN:O	1:C:230:ARG:HG2	2.11	0.51
1:D:14:ALA:CB	1:D:58:VAL:HG12	2.41	0.51
1:D:138:LEU:HD11	1:D:160:LEU:HB3	1.93	0.51
1:B:196:LEU:HD12	1:B:196:LEU:H	1.75	0.51
1:D:27:LYS:O	1:D:37:LEU:HD12	2.11	0.51
1:B:70:LEU:O	1:B:72:HIS:N	2.38	0.51
1:B:165:THR:HB	1:B:166:PRO:HA	1.93	0.51
1:C:135:VAL:HG11	1:C:206:VAL:HG11	1.93	0.51
1:C:59:PRO:HB3	1:C:60:ALA:HB2	1.92	0.50
1:B:218:THR:H	1:B:221:ASP:HB2	1.77	0.50
1:A:135:VAL:HG12	1:A:206:VAL:CG1	2.41	0.50
1:B:28:ALA:O	1:B:29:PHE:CB	2.60	0.50
1:D:48:SER:HA	1:D:115:PRO:HB3	1.93	0.50
1:C:8:VAL:HG22	1:C:102:PHE:HB2	1.94	0.50
1:A:165:THR:HB	1:A:166:PRO:HA	1.95	0.49
1:D:61:ASP:C	1:D:63:THR:H	2.20	0.49
1:D:117:LEU:HD23	1:D:117:LEU:C	2.38	0.49
1:B:224:LEU:HD22	1:B:228:ILE:HD11	1.95	0.49
1:C:60:ALA:CB	1:C:61:ASP:HB3	2.42	0.49
1:C:112:LEU:HD22	1:C:216:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:LEU:HD23	1:D:94:LEU:C	2.38	0.49
1:C:141:THR:HB	1:D:163:VAL:HG13	1.93	0.49
1:D:33:ASP:CB	1:D:230:ARG:HH21	2.26	0.49
1:A:118:VAL:O	1:A:122:VAL:HG23	2.14	0.48
1:C:135:VAL:HG11	1:C:206:VAL:CG1	2.42	0.48
1:D:9:VAL:HG22	1:D:53:THR:HB	1.95	0.48
2:F:15:UNK:CA	2:F:16:UNK:CB	2.91	0.48
1:A:224:LEU:HG	1:B:224:LEU:HG	1.96	0.48
1:A:93:VAL:O	1:A:94:LEU:CB	2.62	0.47
1:A:174:LEU:O	1:A:178:TYR:HD2	1.97	0.47
1:C:76:ILE:N	1:C:76:ILE:HD12	2.29	0.47
1:C:103:VAL:HG23	1:C:171:THR:HB	1.96	0.47
1:C:172:ASP:OD1	1:C:172:ASP:N	2.38	0.47
1:B:13:PRO:HG2	1:B:83:ARG:NH1	2.30	0.47
1:C:60:ALA:H	1:C:61:ASP:CA	2.27	0.47
1:D:229:VAL:HG23	1:D:230:ARG:N	2.30	0.47
1:A:222:LEU:HD12	1:A:222:LEU:HA	1.69	0.47
1:B:196:LEU:H	1:B:196:LEU:CD1	2.28	0.46
1:C:165:THR:CB	1:C:166:PRO:HA	2.44	0.46
1:C:205:GLN:HG3	1:C:206:VAL:H	1.80	0.46
1:D:81:SER:O	1:D:82:ASN:OD1	2.32	0.46
1:A:146:ASP:C	1:A:146:ASP:OD2	2.59	0.46
1:C:94:LEU:CB	1:C:95:SER:CA	2.66	0.46
1:C:117:LEU:HD23	1:C:117:LEU:C	2.41	0.46
1:A:226:GLN:O	1:A:227:ALA:C	2.58	0.46
1:A:163:VAL:HG21	1:B:143:LYS:HG3	1.97	0.46
1:C:109:ALA:HB3	1:C:215:LYS:HG2	1.97	0.46
1:D:134:PRO:HA	1:D:207:VAL:O	2.16	0.46
2:F:15:UNK:HA	2:F:16:UNK:CB	2.45	0.46
1:C:120:ARG:NH1	1:C:208:ASP:O	2.46	0.45
1:D:160:LEU:O	1:D:161:ARG:HD3	2.16	0.45
1:A:58:VAL:O	1:A:79:GLY:N	2.49	0.45
1:C:205:GLN:HG3	1:C:206:VAL:N	2.31	0.45
1:B:44:GLY:HA3	3:B:245:HOH:O	2.15	0.45
1:C:35:GLN:NE2	1:C:39:GLU:HG2	2.32	0.45
1:C:134:PRO:HG2	1:C:164:GLN:HB2	1.97	0.45
1:D:75:MET:O	1:D:76:ILE:HD12	2.17	0.45
1:C:91:LEU:HD12	1:C:91:LEU:HA	1.79	0.45
1:B:56:VAL:HG12	1:B:58:VAL:CG1	2.47	0.45
1:C:42:VAL:O	1:C:46:LEU:HG	2.17	0.45
1:A:9:VAL:CG1	1:A:10:ALA:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.82	0.44
1:D:26:PRO:HG2	1:D:27:LYS:H	1.81	0.44
1:D:94:LEU:HD23	1:D:95:SER:N	2.32	0.44
1:D:138:LEU:HD13	1:D:142:ILE:HG12	1.98	0.44
1:B:32:LEU:HD23	1:B:40:ARG:CD	2.48	0.44
1:D:30:TYR:O	1:D:36:THR:HA	2.16	0.44
1:A:214:PHE:HE2	1:A:221:ASP:HB3	1.82	0.44
1:B:28:ALA:HB2	1:B:108:ALA:HB3	1.98	0.44
1:B:220:LEU:HD12	1:B:220:LEU:HA	1.83	0.44
1:D:146:ASP:OD2	1:D:146:ASP:C	2.61	0.44
1:C:43:ASP:HA	1:C:46:LEU:HD12	2.00	0.44
1:D:170:THR:O	1:D:171:THR:C	2.60	0.44
1:D:90:ALA:O	1:D:93:VAL:O	2.36	0.44
1:B:130:ALA:HA	1:B:170:THR:HG23	1.98	0.43
1:B:146:ASP:OD2	1:B:146:ASP:C	2.60	0.43
1:C:125:LEU:HD11	1:C:168:GLY:HA3	2.00	0.43
1:B:132:VAL:HA	1:B:205:GLN:O	2.18	0.43
1:C:48:SER:HA	1:C:115:PRO:HB3	2.01	0.43
1:A:63:THR:HG23	1:A:64:ASP:N	2.33	0.43
1:A:135:VAL:HG22	1:A:136:LEU:H	1.83	0.43
1:B:229:VAL:HG23	1:B:230:ARG:N	2.33	0.43
1:C:211:PRO:O	1:C:214:PHE:HD1	2.01	0.43
1:C:220:LEU:HD12	1:C:220:LEU:HA	1.82	0.43
1:A:70:LEU:O	1:A:73:ARG:HB2	2.18	0.43
1:D:222:LEU:HD12	1:D:222:LEU:HA	1.77	0.43
1:A:30:TYR:O	1:A:36:THR:HA	2.19	0.43
1:A:88:ASN:HD21	1:A:178:TYR:HB3	1.83	0.43
1:D:106:HIS:HD2	1:D:165:THR:OG1	2.02	0.43
1:A:33:ASP:OD2	1:A:229:VAL:HG11	2.19	0.43
1:A:33:ASP:CG	1:A:33:ASP:O	2.62	0.43
1:D:61:ASP:C	1:D:63:THR:N	2.77	0.43
1:B:94:LEU:HD12	1:B:94:LEU:HA	1.71	0.42
1:B:117:LEU:CD2	1:B:166:PRO:HD2	2.49	0.42
1:D:110:ARG:HD2	1:D:165:THR:OG1	2.19	0.42
1:A:124:ALA:HB3	1:A:132:VAL:HG21	2.01	0.42
1:A:205:GLN:HG3	1:A:206:VAL:N	2.34	0.42
1:D:91:LEU:HD12	1:D:91:LEU:HA	1.82	0.42
1:A:38:ILE:HD12	1:A:38:ILE:HA	1.86	0.42
1:C:87:VAL:C	1:C:89:LEU:N	2.76	0.42
1:C:142:ILE:HD12	1:D:138:LEU:HD21	2.02	0.42
1:A:226:GLN:C	1:A:230:ARG:HD2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:O	1:C:93:VAL:HG23	2.19	0.42
1:A:39:GLU:HG3	1:A:73:ARG:NH1	2.35	0.42
1:B:154:THR:HA	1:B:155:PRO:HD2	1.88	0.42
1:C:35:GLN:HE21	1:C:35:GLN:HB3	1.57	0.42
1:C:60:ALA:HB3	1:C:61:ASP:HB2	2.00	0.42
1:C:32:LEU:O	1:C:33:ASP:C	2.63	0.42
1:C:173:LEU:HD12	1:C:173:LEU:C	2.45	0.42
1:D:83:ARG:NH2	1:D:193:ASP:OD2	2.52	0.41
1:A:39:GLU:HG3	1:A:73:ARG:HH12	1.85	0.41
1:B:181:GLY:HA2	1:B:182:SER:HA	1.82	0.41
1:B:178:TYR:CE2	1:B:196:LEU:CD2	3.04	0.41
1:C:93:VAL:O	1:C:94:LEU:HB2	2.21	0.41
1:A:220:LEU:HD12	1:A:220:LEU:HA	1.85	0.41
1:B:58:VAL:O	1:B:79:GLY:HA3	2.21	0.41
1:B:72:HIS:HA	1:B:73:ARG:C	2.33	0.41
1:B:113:THR:HA	1:B:114:PRO:HD3	1.88	0.41
1:A:75:MET:HE3	1:A:75:MET:HB2	1.97	0.41
1:A:110:ARG:HD2	1:A:165:THR:OG1	2.21	0.41
1:B:72:HIS:CA	1:B:74:ALA:H	2.19	0.41
1:B:218:THR:N	1:B:221:ASP:OD2	2.53	0.41
1:C:224:LEU:O	1:C:225:ALA:C	2.64	0.41
1:D:50:VAL:HG21	1:D:119:ALA:HA	2.02	0.41
1:B:99:GLU:HA	1:B:100:PRO:HD3	1.84	0.41
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.87	0.41
1:D:42:VAL:HG22	1:D:54:VAL:HG11	2.03	0.40
1:A:83:ARG:O	1:A:84:THR:C	2.63	0.40
1:B:126:ARG:HG2	1:B:126:ARG:HH11	1.86	0.40
1:D:13:PRO:HG2	1:D:83:ARG:NH1	2.36	0.40
1:B:28:ALA:HB1	1:B:108:ALA:HB1	2.04	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	195/231 (84%)	179 (92%)	13 (7%)	3 (2%)	8	12
1	B	202/231 (87%)	184 (91%)	14 (7%)	4 (2%)	6	7
1	C	184/231 (80%)	167 (91%)	10 (5%)	7 (4%)	2	2
1	D	199/231 (86%)	182 (92%)	14 (7%)	3 (2%)	8	12
All	All	780/924 (84%)	712 (91%)	51 (6%)	17 (2%)	5	6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	157	ARG
1	B	29	PHE
1	C	33	ASP
1	C	78	ALA
1	C	94	LEU
1	A	33	ASP
1	B	71	GLY
1	B	72	HIS
1	C	61	ASP
1	C	157	ARG
1	B	73	ARG
1	D	94	LEU
1	D	60	ALA
1	C	60	ALA
1	C	155	PRO
1	D	82	ASN

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	142/178 (80%)	123 (87%)	19 (13%)	4	5
1	B	146/178 (82%)	131 (90%)	15 (10%)	7	11
1	C	131/178 (74%)	113 (86%)	18 (14%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	141/178 (79%)	124 (88%)	17 (12%)	5	7
All	All	560/712 (79%)	491 (88%)	69 (12%)	4	6

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	88	ASN
1	A	91	LEU
1	A	92	THR
1	A	105	VAL
1	A	112	LEU
1	A	123	GLU
1	A	138	LEU
1	A	139	SER
1	A	160	LEU
1	A	204	VAL
1	A	206	VAL
1	A	212	LEU
1	A	215	LYS
1	A	219	LYS
1	A	222	LEU
1	A	224	LEU
1	A	229	VAL
1	A	230	ARG
1	B	58	VAL
1	B	91	LEU
1	B	92	THR
1	B	94	LEU
1	B	112	LEU
1	B	135	VAL
1	B	139	SER
1	B	160	LEU
1	B	163	VAL
1	B	171	THR
1	B	204	VAL
1	B	206	VAL
1	B	212	LEU
1	B	224	LEU
1	B	230	ARG
1	C	35	GLN
1	C	53	THR

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Mol	Chain	Res	Type
1	C	88	ASN
1	C	91	LEU
1	C	94	LEU
1	C	112	LEU
1	C	135	VAL
1	C	138	LEU
1	C	139	SER
1	C	171	THR
1	C	172	ASP
1	C	192	ASP
1	C	197	VAL
1	C	204	VAL
1	C	206	VAL
1	C	212	LEU
1	C	215	LYS
1	C	224	LEU
1	D	50	VAL
1	D	77	VAL
1	D	82	ASN
1	D	89	LEU
1	D	91	LEU
1	D	92	THR
1	D	94	LEU
1	D	112	LEU
1	D	135	VAL
1	D	160	LEU
1	D	171	THR
1	D	204	VAL
1	D	206	VAL
1	D	212	LEU
1	D	220	LEU
1	D	224	LEU
1	D	230	ARG

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

Mol	Chain	Res	Type
1	A	68	GLN
1	A	88	ASN
1	A	106	HIS
1	A	179	GLN
1	A	203	GLN

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	226	GLN
1	B	106	HIS
1	B	205	GLN
1	B	226	GLN
1	C	35	GLN
1	C	88	ASN
1	C	106	HIS
1	C	205	GLN
1	C	226	GLN
1	D	106	HIS
1	D	205	GLN
1	D	226	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 oligosaccharides 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	203/231 (87%)	-0.07	3 (1%) 72 68	44, 64, 106, 132	0
1	B	208/231 (90%)	-0.02	7 (3%) 48 44	40, 61, 94, 128	0
1	C	194/231 (83%)	0.08	4 (2%) 63 59	46, 75, 119, 136	0
1	D	205/231 (88%)	-0.07	1 (0%) 87 85	39, 62, 99, 129	0
2	F	0/7	-	-	-	-
All	All	810/931 (87%)	-0.02	15 (1%) 66 62	39, 64, 108, 136	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	VAL	3.3
1	C	178	TYR	3.0
1	C	95	SER	2.8
1	B	28	ALA	2.8
1	A	95	SER	2.7
1	D	191	THR	2.6
1	B	10	ALA	2.4
1	B	96	GLY	2.4
1	B	97	THR	2.3
1	C	26	PRO	2.3
1	A	84	THR	2.2
1	B	196	LEU	2.2
1	A	85	ASP	2.2
1	B	69	ILE	2.1
1	B	183	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.