



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 07:04 PM GMT

PDB ID : 3D3Q
Title : Crystal structure of tRNA delta(2)-isopentenylpyrophosphatetransferase (SE0981) from Staphylococcus epidermidis. Northeast Structural Genomics Consortium target SeR100
Authors : Forouhar, F.; Abashidze, M.; Seetharaman, J.; Mao, L.; Xiao, R.; Maglaqui, M.; Lee, D.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-05-12
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

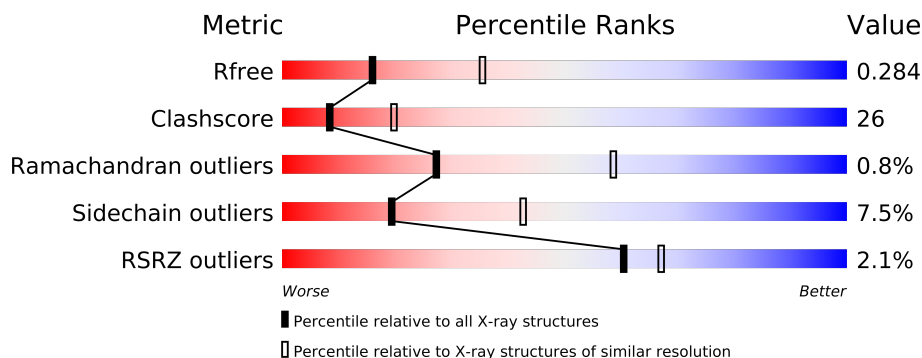
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

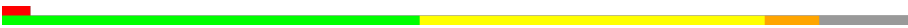
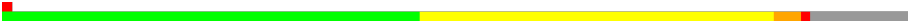
The reported resolution of this entry is 2.70 Å.

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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5011 atoms, of which 0 are hydrogen and 0 are deuterium.

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 tRNA delta(2)-isopentenylpyrophosphatetransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	Se	0	0	0
			2498	1594	432	459	13			
1	B	303	Total	C	N	O	Se	0	0	0
			2469	1577	428	451	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	LEU	-	EXPRESSION TAG	UNP Q8CQL3
A	334	GLU	-	EXPRESSION TAG	UNP Q8CQL3
A	335	HIS	-	EXPRESSION TAG	UNP Q8CQL3
A	336	HIS	-	EXPRESSION TAG	UNP Q8CQL3
A	337	HIS	-	EXPRESSION TAG	UNP Q8CQL3
A	338	HIS	-	EXPRESSION TAG	UNP Q8CQL3
A	339	HIS	-	EXPRESSION TAG	UNP Q8CQL3
A	340	HIS	-	EXPRESSION TAG	UNP Q8CQL3
B	333	LEU	-	EXPRESSION TAG	UNP Q8CQL3
B	334	GLU	-	EXPRESSION TAG	UNP Q8CQL3
B	335	HIS	-	EXPRESSION TAG	UNP Q8CQL3
B	336	HIS	-	EXPRESSION TAG	UNP Q8CQL3
B	337	HIS	-	EXPRESSION TAG	UNP Q8CQL3
B	338	HIS	-	EXPRESSION TAG	UNP Q8CQL3
B	339	HIS	-	EXPRESSION TAG	UNP Q8CQL3
B	340	HIS	-	EXPRESSION TAG	UNP Q8CQL3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	22	Total	O	0	0
			22	22		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.62Å 84.48Å 75.40Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	19.92 – 2.70 28.19 – 2.56	Depositor EDS
% Data completeness (in resolution range)	72.5 (19.92-2.70) 88.3 (28.19-2.56)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.231 , 0.271 0.252 , 0.284	Depositor DCC
R_{free} test set	1683 reflections (8.19%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 38847 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5011	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.49	0/2527	0.88	12/3365 (0.4%)
1	B	0.47	0/2498	0.87	12/3326 (0.4%)
All	All	0.48	0/5025	0.87	24/6691 (0.4%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ARG	NE-CZ-NH1	-13.35	113.63	120.30
1	B	213	ARG	NE-CZ-NH2	-13.25	113.68	120.30
1	A	279	ARG	NE-CZ-NH1	-13.22	113.69	120.30
1	A	297	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	A	279	ARG	NE-CZ-NH2	12.98	126.79	120.30
1	B	213	ARG	NE-CZ-NH1	12.93	126.76	120.30
1	A	213	ARG	NE-CZ-NH1	-12.89	113.86	120.30
1	B	279	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	B	297	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	A	207	ARG	NE-CZ-NH2	12.60	126.60	120.30
1	A	213	ARG	NE-CZ-NH2	12.31	126.45	120.30
1	A	207	ARG	NE-CZ-NH1	-12.15	114.22	120.30
1	A	297	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	B	207	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	B	279	ARG	NE-CZ-NH1	11.81	126.21	120.30
1	B	207	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	B	297	ARG	CD-NE-CZ	7.00	133.41	123.60
1	A	279	ARG	CD-NE-CZ	6.76	133.06	123.60
1	B	279	ARG	CD-NE-CZ	6.57	132.80	123.60
1	A	297	ARG	CD-NE-CZ	6.52	132.72	123.60
1	B	207	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	213	ARG	CD-NE-CZ	5.99	131.99	123.60
1	B	213	ARG	CD-NE-CZ	5.88	131.82	123.60
1	A	207	ARG	CD-NE-CZ	5.86	131.81	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2498	0	2571	134	0
1	B	2469	0	2544	129	0
2	A	22	0	0	3	0
2	B	22	0	0	8	0
All	All	5011	0	5115	263	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (263) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:138:LEU:HD22	1:B:141:LEU:HD11	1.48	0.95
1:B:66:MSE:HE2	1:B:81:PHE:HD1	1.42	0.82
1:A:66:MSE:HE2	1:A:81:PHE:HD1	1.44	0.82
1:A:113:LEU:HD22	1:A:198:THR:HG21	1.61	0.81
1:B:113:LEU:HD22	1:B:198:THR:HG21	1.64	0.79
1:A:183:LEU:O	1:A:183:LEU:HD22	1.83	0.77
1:B:136:LYS:HE2	1:B:139:GLU:CD	2.04	0.77
1:B:113:LEU:HD12	1:B:288:MSE:HE1	1.66	0.76
1:B:136:LYS:HA	1:B:139:GLU:HG3	1.65	0.76
1:A:205:MSE:HE2	1:A:210:LEU:HA	1.67	0.76
1:A:262:MSE:HE2	1:A:266:VAL:HG23	1.68	0.75
1:A:113:LEU:HD12	1:A:288:MSE:HE1	1.68	0.75
1:B:205:MSE:HE2	1:B:210:LEU:HA	1.68	0.75
1:A:175:TYR:O	1:A:179:THR:HG22	1.87	0.74
1:A:205:MSE:HE1	1:A:213:ARG:HD3	1.68	0.74
1:B:262:MSE:HE2	1:B:266:VAL:HG23	1.69	0.73
1:A:262:MSE:HE2	1:A:266:VAL:CG2	2.19	0.73
1:A:7:PRO:HG2	1:A:196:TYR:HD2	1.54	0.72
1:B:252:LEU:O	1:B:255:VAL:HG12	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:ASN:HB2	1:A:193:THR:HG22	1.71	0.71
1:B:204:GLU:HG2	1:B:205:MSE:N	2.05	0.71
1:B:262:MSE:HE2	1:B:266:VAL:CG2	2.21	0.71
1:B:66:MSE:HE1	1:B:76:PHE:HZ	1.55	0.71
1:B:119:GLU:HG2	1:B:181:LYS:NZ	2.05	0.70
1:B:305:ASP:O	1:B:308:THR:HG22	1.91	0.70
1:A:11:VAL:HG22	1:A:101:ILE:HD11	1.73	0.70
1:B:204:GLU:HG2	1:B:205:MSE:H	1.57	0.70
1:A:305:ASP:O	1:A:308:THR:HG22	1.91	0.70
1:B:271:GLN:HG2	1:B:275:GLN:HE21	1.56	0.69
1:A:66:MSE:HE1	1:A:76:PHE:HZ	1.55	0.69
1:A:218:VAL:O	1:A:222:LEU:HD23	1.93	0.69
1:A:230:VAL:HG23	1:A:256:ILE:HD11	1.74	0.69
1:B:218:VAL:O	1:B:222:LEU:HD23	1.92	0.69
1:B:249:TYR:O	1:B:253:VAL:HG23	1.93	0.68
1:A:252:LEU:O	1:A:255:VAL:HG12	1.93	0.68
1:A:182:LEU:HD23	1:A:182:LEU:H	1.58	0.68
1:A:204:GLU:HG2	1:A:205:MSE:N	2.10	0.67
1:A:271:GLN:HG2	1:A:275:GLN:HE21	1.58	0.67
1:B:297:ARG:HD2	2:B:350:HOH:O	1.95	0.67
1:B:230:VAL:HG23	1:B:256:ILE:HD11	1.76	0.67
1:A:204:GLU:HG2	1:A:205:MSE:H	1.60	0.66
1:A:82:LYS:O	1:A:86:GLU:HG3	1.96	0.66
1:B:136:LYS:HE2	1:B:139:GLU:OE1	1.96	0.66
1:B:132:LYS:HD2	1:B:132:LYS:O	1.96	0.65
1:A:150:LEU:HD13	1:A:158:ALA:HB2	1.79	0.64
1:A:179:THR:HG23	1:A:181:LYS:H	1.62	0.64
1:B:82:LYS:O	1:B:86:GLU:HG3	1.98	0.64
1:A:249:TYR:O	1:A:253:VAL:HG23	1.97	0.64
1:A:232:HIS:HB3	2:A:351:HOH:O	1.98	0.63
1:A:12:ILE:HG23	1:A:201:ILE:HD11	1.81	0.63
1:B:6:LYS:N	1:B:7:PRO:HD2	2.13	0.63
1:A:127:LYS:HE2	1:A:130:GLN:HE21	1.64	0.63
1:B:217:ARG:O	1:B:221:MSE:HG3	1.99	0.63
1:B:11:VAL:HG22	1:B:101:ILE:HD11	1.82	0.62
1:A:217:ARG:O	1:A:221:MSE:HG3	1.98	0.62
1:B:168:ARG:HE	1:B:171:ARG:HH11	1.48	0.61
1:B:36:ILE:HB	1:B:101:ILE:HG22	1.81	0.61
1:B:6:LYS:NZ	1:B:6:LYS:HB2	2.15	0.61
1:B:186:ARG:HD3	1:B:190:GLN:CD	2.21	0.61
1:B:94:ARG:HD3	2:B:341:HOH:O	1.99	0.60
1:B:141:LEU:O	1:B:143:ASN:N	2.33	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:PRO:HG2	1:A:196:TYR:CD2	2.37	0.60
1:B:12:ILE:HG23	1:B:201:ILE:HD11	1.83	0.60
1:A:36:ILE:HB	1:A:101:ILE:HG22	1.83	0.59
1:B:145:LYS:HD3	1:B:145:LYS:O	2.02	0.59
1:A:10:ILE:CD1	1:A:199:LEU:HD23	2.33	0.58
1:B:188:LYS:HE3	2:B:346:HOH:O	2.04	0.57
1:B:174:GLU:HG2	1:B:178:LYS:HE3	1.86	0.57
1:A:205:MSE:HE1	1:A:213:ARG:CD	2.34	0.57
1:B:80:GLU:HA	1:B:80:GLU:OE2	2.05	0.56
1:B:205:MSE:HE2	1:B:210:LEU:CA	2.34	0.56
1:A:205:MSE:HE2	1:A:210:LEU:CA	2.33	0.56
1:A:8:PHE:CE1	1:A:314:ARG:HG3	2.40	0.56
1:A:252:LEU:CD2	1:A:262:MSE:HE1	2.36	0.56
1:A:270:LYS:O	1:A:274:ARG:HG3	2.06	0.56
1:B:299:SER:H	1:B:302:MSE:HB2	1.72	0.55
1:B:168:ARG:HA	1:B:171:ARG:HD2	1.89	0.55
1:B:216:LYS:O	1:B:220:ILE:HG13	2.06	0.55
1:B:142:ASN:C	1:B:144:ASN:H	2.10	0.55
1:B:254:PRO:HB2	1:B:260:ILE:HG21	1.88	0.55
1:A:209:THR:O	1:A:213:ARG:HG3	2.06	0.55
1:A:254:PRO:HB2	1:A:260:ILE:HG21	1.89	0.55
1:B:176:TYR:HD2	1:B:177:LEU:HD12	1.70	0.55
1:A:115:ASN:ND2	1:A:195:ASN:HD21	2.04	0.55
1:A:80:GLU:OE2	1:A:80:GLU:HA	2.06	0.54
1:B:270:LYS:O	1:B:274:ARG:HG3	2.06	0.54
1:B:254:PRO:HB2	1:B:260:ILE:CG2	2.37	0.54
1:B:237:GLY:HA2	2:B:349:HOH:O	2.06	0.54
1:B:45:GLN:HA	1:B:68:ASP:OD1	2.07	0.54
1:B:6:LYS:N	1:B:7:PRO:CD	2.70	0.54
1:A:254:PRO:HB2	1:A:260:ILE:CG2	2.38	0.54
1:A:123:ILE:N	1:A:123:ILE:HD13	2.23	0.54
1:A:216:LYS:O	1:A:220:ILE:HG13	2.08	0.54
1:B:141:LEU:C	1:B:143:ASN:H	2.10	0.53
1:A:94:ARG:HG2	1:A:94:ARG:HH21	1.73	0.53
1:A:299:SER:H	1:A:302:MSE:HB2	1.73	0.53
1:B:251:GLU:O	1:B:254:PRO:HD2	2.08	0.53
1:B:65:TYR:O	1:B:66:MSE:HB2	2.09	0.53
1:A:56:THR:HA	1:A:59:MSE:HE3	1.91	0.53
1:A:176:TYR:O	1:A:180:LYS:N	2.38	0.53
1:B:119:GLU:HG2	1:B:181:LYS:HZ3	1.74	0.53
1:A:127:LYS:HE2	1:A:130:GLN:NE2	2.23	0.53
1:A:247:ILE:HD11	1:A:273:SER:OG	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:294:ASN:H	1:B:298:MSE:HE3	1.73	0.52
1:A:45:GLN:HA	1:A:68:ASP:OD1	2.08	0.52
1:A:239:GLU:O	1:A:240:ALA:HB3	2.08	0.52
1:B:252:LEU:CD2	1:B:262:MSE:HE1	2.39	0.52
1:B:164:ASN:O	1:B:166:ARG:N	2.39	0.52
1:B:239:GLU:O	1:B:240:ALA:HB3	2.10	0.52
1:B:131:VAL:O	1:B:135:LEU:HG	2.09	0.52
1:B:294:ASN:N	1:B:298:MSE:HE3	2.25	0.52
1:B:7:PRO:HG2	1:B:196:TYR:HD2	1.74	0.51
1:B:35:ILE:HA	1:B:100:ILE:O	2.11	0.51
1:A:66:MSE:HE2	1:A:81:PHE:CD1	2.36	0.51
1:A:294:ASN:H	1:A:298:MSE:HE3	1.75	0.51
1:B:94:ARG:HH21	1:B:94:ARG:HG2	1.75	0.50
1:A:83:LYS:HE2	1:A:87:LYS:NZ	2.25	0.50
1:B:88:TYR:O	1:B:92:ILE:HG13	2.12	0.50
1:A:182:LEU:HB2	1:A:185:SER:HB2	1.93	0.50
1:B:294:ASN:ND2	1:B:296:GLU:H	2.10	0.50
1:B:69:ILE:HG13	1:B:70:LEU:HG	1.94	0.50
1:A:65:TYR:O	1:A:66:MSE:HB2	2.11	0.50
1:A:227:PHE:HE2	1:A:255:VAL:HG13	1.77	0.50
1:B:105:THR:O	1:B:109:ILE:HG12	2.12	0.50
1:A:134:LYS:HG2	2:A:359:HOH:O	2.10	0.50
1:A:141:LEU:HD23	1:A:146:LEU:HA	1.94	0.50
1:A:253:VAL:HB	1:A:254:PRO:HD3	1.94	0.49
1:A:109:ILE:O	1:A:113:LEU:HG	2.12	0.49
1:B:109:ILE:O	1:B:113:LEU:HG	2.12	0.49
1:B:119:GLU:HG2	1:B:181:LYS:HZ1	1.75	0.49
1:A:144:ASN:O	1:A:148:GLU:HG2	2.12	0.49
1:B:10:ILE:CD1	1:B:199:LEU:HD23	2.43	0.49
1:A:11:VAL:HG13	1:A:101:ILE:HG13	1.94	0.49
1:A:134:LYS:O	1:A:138:LEU:HG	2.12	0.49
1:A:294:ASN:N	1:A:298:MSE:HE3	2.27	0.49
1:B:227:PHE:HE2	1:B:255:VAL:HG13	1.76	0.49
1:B:281:LEU:CD1	1:B:285:LYS:HD2	2.42	0.49
1:B:66:MSE:HE2	1:B:81:PHE:CD1	2.34	0.49
1:B:297:ARG:HG2	1:B:297:ARG:O	2.12	0.49
1:A:183:LEU:C	1:A:183:LEU:HD13	2.32	0.49
1:B:176:TYR:CD2	1:B:177:LEU:HD12	2.46	0.49
1:B:239:GLU:CG	2:B:348:HOH:O	2.60	0.49
1:B:262:MSE:O	1:B:266:VAL:HG23	2.13	0.49
1:B:83:LYS:HE2	1:B:87:LYS:NZ	2.28	0.49
1:B:91:ASP:OD2	1:B:95:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:ILE:HG13	1:A:70:LEU:HG	1.95	0.49
1:B:66:MSE:HE1	1:B:76:PHE:CZ	2.43	0.48
1:A:11:VAL:CG2	1:A:101:ILE:HD11	2.41	0.48
1:B:247:ILE:HD11	1:B:273:SER:OG	2.13	0.48
1:B:138:LEU:CD2	1:B:141:LEU:HD11	2.30	0.48
1:A:183:LEU:C	1:A:183:LEU:HD22	2.33	0.48
1:B:132:LYS:HD2	1:B:132:LYS:C	2.33	0.48
1:A:105:THR:O	1:A:109:ILE:HG12	2.14	0.48
1:A:262:MSE:O	1:A:266:VAL:HG23	2.13	0.48
1:A:55:THR:OG1	1:A:58:GLU:HG3	2.12	0.48
1:A:213:ARG:NH2	1:A:295:LYS:HE3	2.29	0.48
1:A:115:ASN:CB	1:A:193:THR:HG22	2.40	0.48
1:B:11:VAL:HG13	1:B:101:ILE:HG13	1.94	0.48
1:B:56:THR:HA	1:B:59:MSE:HE3	1.95	0.48
1:A:179:THR:OG1	1:A:181:LYS:HE2	2.14	0.47
1:A:35:ILE:HA	1:A:100:ILE:O	2.15	0.47
1:B:6:LYS:HB2	1:B:6:LYS:HZ2	1.79	0.47
1:A:10:ILE:HD13	1:A:199:LEU:HB3	1.97	0.47
1:B:133:LEU:O	1:B:136:LYS:HB3	2.14	0.47
1:B:186:ARG:O	1:B:190:GLN:HG3	2.14	0.47
1:B:95:ARG:HH21	1:B:95:ARG:HG3	1.79	0.47
1:B:213:ARG:NH2	1:B:295:LYS:HE3	2.30	0.47
1:A:88:TYR:O	1:A:92:ILE:HG13	2.14	0.47
1:B:252:LEU:O	1:B:256:ILE:HG13	2.15	0.46
1:A:125:GLU:HA	1:A:125:GLU:OE1	2.15	0.46
1:B:47:MSE:SE	1:B:243:SER:HB2	2.65	0.46
1:B:294:ASN:HD22	1:B:294:ASN:C	2.18	0.46
1:A:294:ASN:HD22	1:A:294:ASN:C	2.19	0.46
1:B:55:THR:OG1	1:B:58:GLU:HG3	2.16	0.46
1:B:189:VAL:O	1:B:193:THR:HG23	2.14	0.46
1:B:176:TYR:O	1:B:180:LYS:HA	2.15	0.46
1:A:294:ASN:ND2	1:A:296:GLU:H	2.13	0.46
1:A:95:ARG:HG3	1:A:95:ARG:HH21	1.80	0.46
1:B:181:LYS:O	1:B:182:LEU:HD23	2.15	0.46
1:A:281:LEU:CD1	1:A:285:LYS:HD2	2.46	0.46
1:A:179:THR:OG1	1:A:181:LYS:HG2	2.16	0.45
1:B:83:LYS:HE2	1:B:87:LYS:HZ1	1.82	0.45
1:A:66:MSE:HE1	1:A:76:PHE:CZ	2.43	0.45
1:A:175:TYR:CD2	1:A:183:LEU:HB2	2.51	0.45
1:B:147:HIS:HE1	1:B:161:ILE:O	2.00	0.45
1:A:252:LEU:O	1:A:256:ILE:HG13	2.16	0.45
1:B:24:SER:HB3	1:B:35:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:253:VAL:HB	1:B:254:PRO:HD3	1.97	0.45
1:A:128:MSE:O	1:A:132:LYS:HB2	2.16	0.45
1:A:11:VAL:HG22	1:A:101:ILE:CD1	2.46	0.45
1:B:252:LEU:HD22	1:B:262:MSE:HE1	1.99	0.45
1:A:238:PHE:O	1:A:244:MSE:HG3	2.17	0.44
1:B:155:LYS:O	1:B:159:LYS:HB2	2.17	0.44
1:A:252:LEU:HD22	1:A:262:MSE:HE1	1.98	0.44
1:B:174:GLU:CG	1:B:178:LYS:HE3	2.48	0.44
1:B:264:ASN:O	1:B:267:GLU:HB3	2.16	0.44
1:A:251:GLU:O	1:A:254:PRO:HD2	2.17	0.44
1:A:83:LYS:HE2	1:A:87:LYS:HZ1	1.83	0.44
1:B:85:ALA:O	1:B:89:ILE:HG13	2.18	0.44
1:B:238:PHE:O	1:B:244:MSE:HG3	2.17	0.44
1:B:168:ARG:NH1	1:B:183:LEU:HD21	2.33	0.44
1:A:15:PRO:HG2	1:A:18:SER:HB3	2.00	0.44
1:B:253:VAL:N	1:B:254:PRO:CD	2.81	0.43
1:A:66:MSE:CE	1:A:76:PHE:HZ	2.29	0.43
1:A:230:VAL:CG2	1:A:256:ILE:HD11	2.47	0.43
1:A:11:VAL:HB	1:A:200:LEU:HD12	2.01	0.43
1:B:281:LEU:O	1:B:285:LYS:HG3	2.18	0.43
1:A:171:ARG:HH11	1:A:175:TYR:HB2	1.84	0.43
1:A:53:LYS:HE3	1:A:53:LYS:HB2	1.81	0.43
1:B:162:HIS:CE1	1:B:163:PRO:HG2	2.53	0.43
1:B:262:MSE:HE3	1:B:262:MSE:HA	2.00	0.43
1:A:131:VAL:HG21	1:A:178:LYS:HG2	2.01	0.43
1:B:15:PRO:HG2	1:B:18:SER:HB3	2.01	0.43
1:A:189:VAL:HG23	1:A:190:GLN:N	2.34	0.43
1:A:131:VAL:HG21	1:A:178:LYS:CG	2.48	0.43
1:A:313:LYS:HA	1:A:313:LYS:HD3	1.86	0.43
1:A:26:GLU:HB3	1:A:304:LEU:HD22	2.00	0.43
1:B:227:PHE:O	1:B:231:GLN:HG3	2.19	0.42
1:B:11:VAL:CG2	1:B:101:ILE:HD11	2.49	0.42
1:A:131:VAL:HG22	1:A:177:LEU:HB3	2.01	0.42
1:A:140:HIS:CD2	1:A:141:LEU:HD12	2.54	0.42
1:A:200:LEU:HD21	1:A:288:MSE:HE3	2.01	0.42
1:A:227:PHE:O	1:A:230:VAL:HG22	2.19	0.42
1:B:31:PHE:O	1:B:32:ASN:C	2.57	0.42
1:A:136:LYS:HG3	1:A:139:GLU:OE1	2.19	0.42
1:B:200:LEU:HD21	1:B:288:MSE:HE3	2.02	0.42
1:A:24:SER:HB3	1:A:35:ILE:HD13	2.00	0.42
1:A:19:GLY:HA2	1:A:22:GLU:OE2	2.19	0.42
1:A:237:GLY:C	1:A:239:GLU:H	2.24	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:MSE:HE3	1:A:233:LEU:HD13	2.01	0.42
1:A:200:LEU:CD2	1:A:288:MSE:HE3	2.50	0.41
1:A:142:ASN:ND2	1:A:145:LYS:HB2	2.35	0.41
1:A:125:GLU:O	1:A:128:MSE:HB2	2.20	0.41
1:A:281:LEU:O	1:A:285:LYS:HG3	2.20	0.41
1:B:53:LYS:HB2	1:B:53:LYS:HE3	1.81	0.41
1:A:130:GLN:O	1:A:134:LYS:HB2	2.20	0.41
1:B:188:LYS:HG3	2:B:346:HOH:O	2.19	0.41
1:B:17:ALA:O	1:B:213:ARG:NH2	2.53	0.41
1:A:31:PHE:O	1:A:32:ASN:C	2.58	0.41
1:B:118:PHE:HD1	2:B:361:HOH:O	2.03	0.41
1:B:10:ILE:HD13	1:B:199:LEU:HB3	2.02	0.41
1:A:205:MSE:HE2	1:A:210:LEU:N	2.36	0.41
1:B:143:ASN:HA	1:B:166:ARG:NH2	2.35	0.41
1:A:115:ASN:C	1:A:193:THR:HG21	2.40	0.41
1:B:199:LEU:HD11	1:B:310:GLN:HG2	2.02	0.41
1:B:227:PHE:O	1:B:230:VAL:HG22	2.21	0.41
1:B:6:LYS:HB2	1:B:6:LYS:HZ3	1.85	0.41
1:B:142:ASN:O	1:B:144:ASN:N	2.54	0.41
1:A:91:ASP:OD2	1:A:95:ARG:NH2	2.54	0.41
1:A:85:ALA:O	1:A:89:ILE:HG13	2.20	0.41
1:A:40:SER:HB3	1:A:108:TYR:CE1	2.56	0.41
1:A:253:VAL:N	1:A:254:PRO:CD	2.84	0.40
1:A:199:LEU:HD11	1:A:310:GLN:HG2	2.03	0.40
1:A:141:LEU:HG	1:A:145:LYS:HD3	2.03	0.40
1:A:134:LYS:HD3	1:A:134:LYS:O	2.21	0.40
1:B:240:ALA:N	2:B:348:HOH:O	2.24	0.40
1:B:19:GLY:HA2	1:B:22:GLU:OE2	2.21	0.40
1:A:175:TYR:HD2	1:A:183:LEU:HB2	1.86	0.40
1:A:227:PHE:O	1:A:231:GLN:HG3	2.22	0.40
1:A:82:LYS:HG2	1:A:86:GLU:OE2	2.22	0.40
1:B:247:ILE:CD1	1:B:273:SER:HA	2.52	0.40
1:A:143:ASN:HA	1:A:143:ASN:HD22	1.54	0.40
1:A:214:ILE:HA	2:A:354:HOH:O	2.21	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	303/340 (89%)	281 (93%)	20 (7%)	2 (1%)	30	62
1	B	299/340 (88%)	277 (93%)	19 (6%)	3 (1%)	22	51
All	All	602/680 (88%)	558 (93%)	39 (6%)	5 (1%)	27	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	142	ASN
1	A	32	ASN
1	A	118	PHE
1	B	32	ASN
1	B	165	ASN

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	275/293 (94%)	250 (91%)	25 (9%)	14	30
1	B	271/293 (92%)	255 (94%)	16 (6%)	28	56
All	All	546/586 (93%)	505 (92%)	41 (8%)	19	43

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	110	GLN
1	A	118	PHE
1	A	123	ILE

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Mol	Chain	Res	Type
1	A	127	LYS
1	A	128	MSE
1	A	130	GLN
1	A	140	HIS
1	A	143	ASN
1	A	150	LEU
1	A	157	SER
1	A	171	ARG
1	A	177	LEU
1	A	180	LYS
1	A	182	LEU
1	A	183	LEU
1	A	193	THR
1	A	247	ILE
1	A	267	GLU
1	A	280	GLN
1	A	281	LEU
1	A	294	ASN
1	A	297	ARG
1	A	308	THR
1	A	310	GLN
1	B	48	ASP
1	B	110	GLN
1	B	132	LYS
1	B	142	ASN
1	B	156	GLU
1	B	168	ARG
1	B	188	LYS
1	B	191	GLN
1	B	247	ILE
1	B	267	GLU
1	B	280	GLN
1	B	281	LEU
1	B	294	ASN
1	B	297	ARG
1	B	308	THR
1	B	310	GLN

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

Mol	Chain	Res	Type
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	115	ASN
1	A	130	GLN
1	A	143	ASN
1	A	147	HIS
1	A	164	ASN
1	A	228	ASN
1	A	264	ASN
1	A	271	GLN
1	A	275	GLN
1	A	286	ASN
1	A	294	ASN
1	A	310	GLN
1	B	110	GLN
1	B	115	ASN
1	B	147	HIS
1	B	164	ASN
1	B	191	GLN
1	B	228	ASN
1	B	236	GLN
1	B	264	ASN
1	B	271	GLN
1	B	275	GLN
1	B	294	ASN
1	B	310	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	307/340 (90%)	0.27	10 (3%)	44 49	30, 46, 63, 79	0
1	B	303/340 (89%)	0.25	3 (0%)	79 83	31, 47, 60, 82	0
All	All	610/680 (89%)	0.26	13 (2%)	60 67	30, 47, 62, 82	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	PHE	4.0
1	B	79	TYR	4.0
1	A	119	GLU	3.1
1	A	128	MSE	2.8
1	A	32	ASN	2.5
1	B	126	ASP	2.4
1	A	160	ASP	2.3
1	A	232	HIS	2.3
1	A	101	ILE	2.2
1	B	142	ASN	2.2
1	A	153	PHE	2.1
1	A	315	SER	2.1
1	A	182	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.