



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:26 PM UTC

PDB ID : 8IHE / pdb_00008ihe
Title : Rv1122(gnd2) in Mycobacterium tuberculosis
Authors : Chen, Y.J.; Su, D.
Deposited on : 2023-02-22
Resolution : 2.74 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

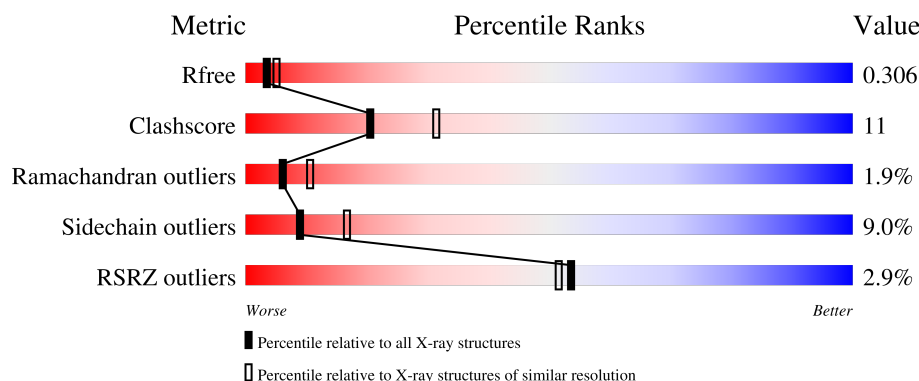
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	340	2% 69% 24% 5% .
1	B	340	% 71% 21% 5% .
1	C	340	% 72% 22% ...
1	D	340	7% 57% 34% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9862 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.

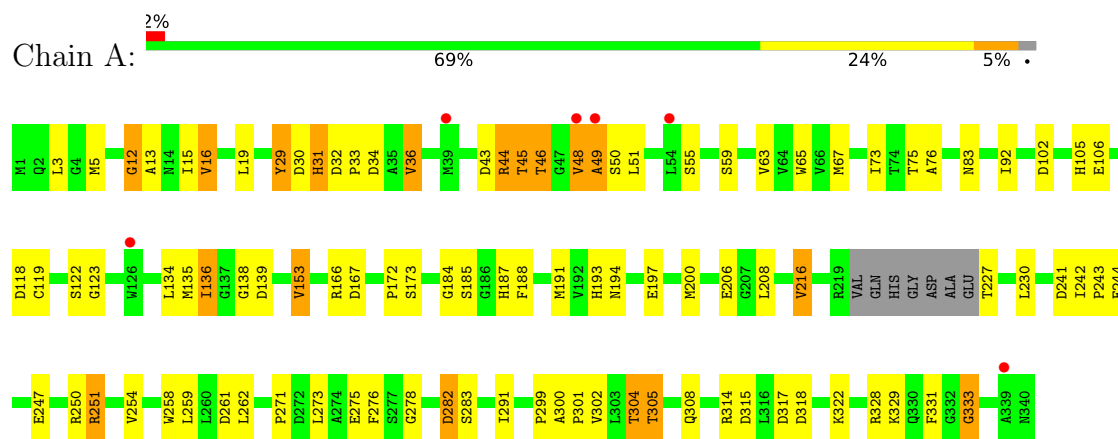
- Molecule 1 is a protein called Probable 6-phosphogluconate dehydrogenase,decarboxylating Gnd2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2500	1558	451	475	16			
1	B	323	Total	C	N	O	S	0	0	0
			2431	1518	437	460	16			
1	C	331	Total	C	N	O	S	0	0	0
			2486	1551	448	471	16			
1	D	325	Total	C	N	O	S	0	0	0
			2445	1527	439	463	16			

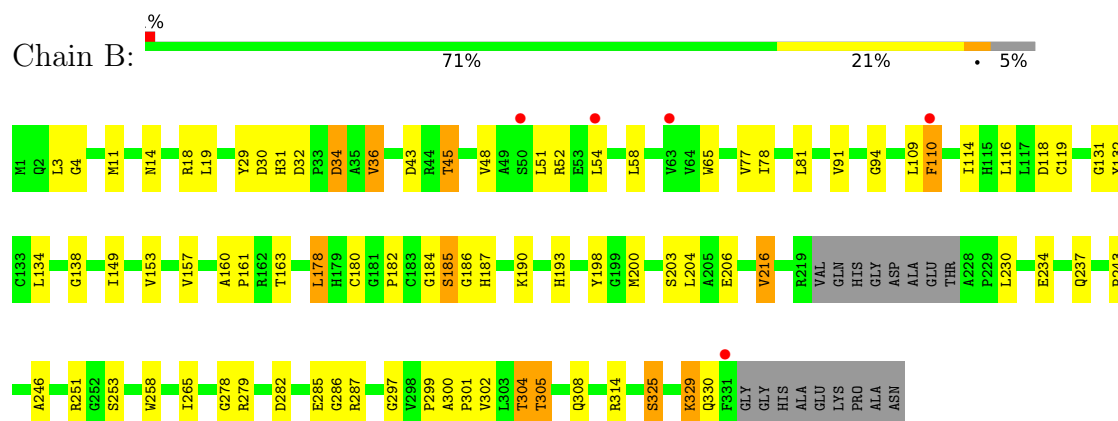
3 Residue-property plots [i](#)

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

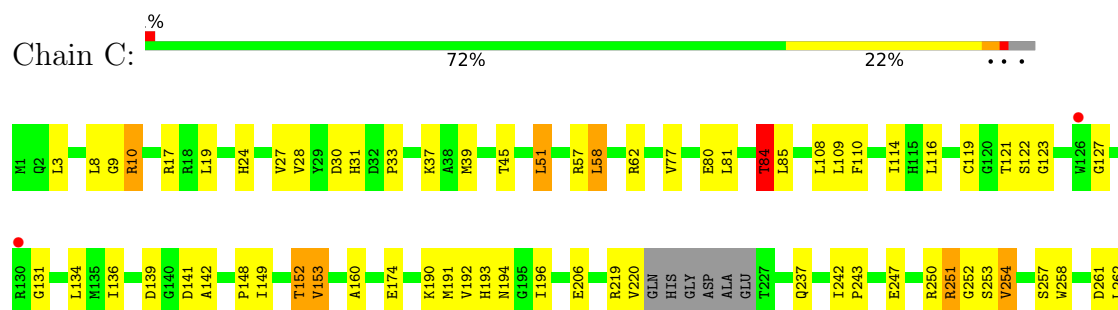
- Molecule 1: Probable 6-phosphogluconate dehydrogenase,decarboxylating Gnd2

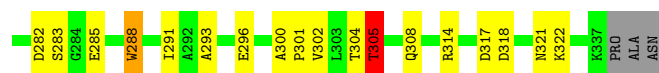


- Molecule 1: Probable 6-phosphogluconate dehydrogenase,decarboxylating Gnd2

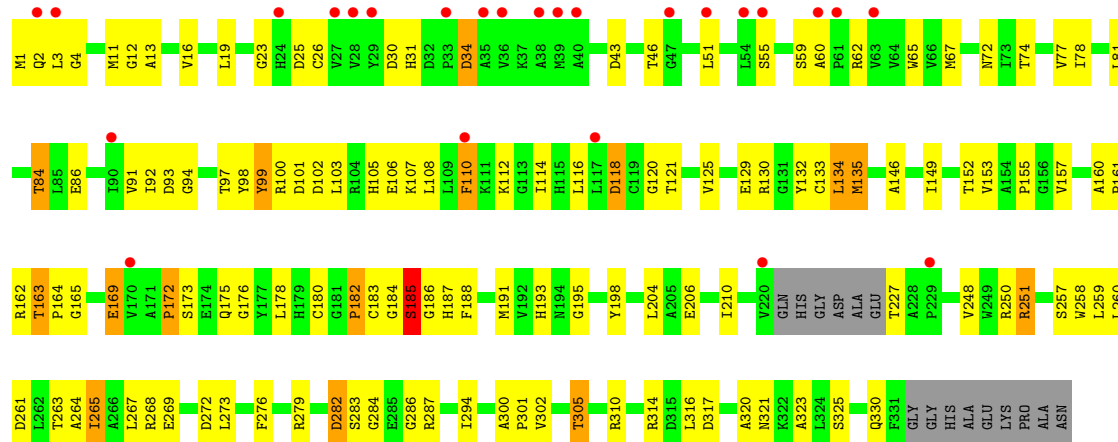


- Molecule 1: Probable 6-phosphogluconate dehydrogenase,decarboxylating Gnd2





- Molecule 1: Probable 6-phosphogluconate dehydrogenase,decarboxylating Gnd2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.99Å 107.25Å 137.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.83 – 2.74 26.83 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.2 (26.83-2.74) 99.2 (26.83-2.74)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.216 , 0.307 0.220 , 0.306	Depositor DCC
R_{free} test set	1842 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9862	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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	1.16	3/2550 (0.1%)	1.59	15/3454 (0.4%)
1	B	1.13	1/2479 (0.0%)	1.56	14/3359 (0.4%)
1	C	1.15	1/2535 (0.0%)	1.62	4/3434 (0.1%)
1	D	1.16	0/2493	1.55	3/3379 (0.1%)
All	All	1.15	5/10057 (0.0%)	1.58	36/13626 (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	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	MET	C-O	6.01	1.30	1.24
1	A	304	THR	C-O	-5.76	1.17	1.24
1	C	261	ASP	C-O	5.52	1.30	1.24
1	B	299	PRO	C-O	-5.33	1.18	1.23
1	A	136	ILE	C-O	5.08	1.29	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ASP	CA-CB-CG	7.72	120.32	112.60
1	A	241	ASP	CA-C-N	7.37	124.88	120.24
1	A	241	ASP	C-N-CA	7.37	124.88	120.24
1	C	305	THR	N-CA-C	-7.02	104.18	112.89
1	B	203	SER	CA-C-N	6.32	129.04	120.44
1	B	203	SER	C-N-CA	6.32	129.04	120.44
1	B	131	GLY	CA-C-O	-6.14	117.99	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	GLY	CA-C-O	-5.93	116.60	121.76
1	D	118	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	325	SER	CA-C-N	5.77	128.01	120.28
1	B	325	SER	C-N-CA	5.77	128.01	120.28
1	D	193	HIS	N-CA-C	-5.73	104.40	111.33
1	B	279	ARG	CB-CA-C	5.67	120.64	111.05
1	B	304	THR	CA-C-N	5.55	127.99	120.38
1	B	304	THR	C-N-CA	5.55	127.99	120.38
1	A	83	ASN	CA-C-N	5.32	127.72	120.54
1	A	83	ASN	C-N-CA	5.32	127.72	120.54
1	C	261	ASP	CA-C-N	5.26	127.33	120.28
1	C	261	ASP	C-N-CA	5.26	127.33	120.28
1	B	265	ILE	CA-C-N	5.17	127.46	120.38
1	B	265	ILE	C-N-CA	5.17	127.46	120.38
1	A	259	LEU	CA-C-O	-5.12	115.10	120.63
1	A	33	PRO	CA-C-N	5.12	127.39	120.38
1	A	33	PRO	C-N-CA	5.12	127.39	120.38
1	A	12	GLY	CA-C-N	5.12	127.90	120.79
1	A	12	GLY	C-N-CA	5.12	127.90	120.79
1	B	246	ALA	CA-C-N	5.12	127.40	120.44
1	B	246	ALA	C-N-CA	5.12	127.40	120.44
1	A	139	ASP	CA-C-N	5.07	125.71	120.03
1	A	139	ASP	C-N-CA	5.07	125.71	120.03
1	B	110	PHE	N-CA-C	-5.05	107.06	113.18
1	D	162	ARG	CB-CA-C	5.04	119.79	109.76
1	A	282	ASP	CA-C-O	-5.03	115.56	121.44
1	C	288	TRP	O-C-N	5.02	127.87	122.15
1	B	149	ILE	N-CA-C	-5.01	105.71	110.42
1	A	331	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ASP	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	2500	0	2448	63	0
1	B	2431	0	2386	60	0
1	C	2486	0	2439	63	0
1	D	2445	0	2402	77	0
All	All	9862	0	9675	218	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 11.

All (218) 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:D:169:GLU:HA	1:D:169:GLU:OE2	1.69	0.91
1:A:305:THR:HG21	1:B:301:PRO:HB2	1.52	0.91
1:D:102:ASP:OD2	1:D:187:HIS:ND1	2.06	0.89
1:C:3:LEU:HD22	1:C:19:LEU:HD13	1.60	0.83
1:D:130:ARG:O	1:D:155:PRO:HB3	1.79	0.82
1:B:134:LEU:HD11	1:B:153:VAL:HG23	1.62	0.81
1:B:134:LEU:HD11	1:B:153:VAL:CG2	2.11	0.80
1:A:302:VAL:HG22	1:B:305:THR:HG22	1.64	0.80
1:B:43:ASP:O	1:B:45:THR:OG1	2.00	0.80
1:A:305:THR:CG2	1:B:301:PRO:HB2	2.13	0.79
1:B:234:GLU:HA	1:B:237:GLN:HE21	1.49	0.78
1:D:134:LEU:HD11	1:D:153:VAL:HG23	1.68	0.76
1:C:302:VAL:HG13	1:D:302:VAL:HG13	1.69	0.75
1:A:188:PHE:O	1:A:191:MET:HB3	1.88	0.74
1:C:148:PRO:O	1:C:152:THR:OG1	2.05	0.74
1:C:301:PRO:O	1:C:305:THR:HB	1.90	0.71
1:C:134:LEU:HD11	1:C:153:VAL:HG22	1.72	0.70
1:A:134:LEU:HD11	1:A:153:VAL:CG2	2.21	0.70
1:D:81:LEU:HA	1:D:84:THR:HG22	1.74	0.69
1:D:30:ASP:OD1	1:D:31:HIS:N	2.26	0.68
1:D:301:PRO:O	1:D:305:THR:HB	1.94	0.68
1:A:119:CYS:SG	1:A:134:LEU:HD22	2.34	0.67
1:A:278:GLY:HA2	1:D:321:ASN:HB3	1.76	0.67
1:C:300:ALA:HA	1:D:206:GLU:OE2	1.96	0.65
1:C:160:ALA:HB3	1:D:251:ARG:HE	1.62	0.65
1:B:301:PRO:O	1:B:305:THR:HB	1.96	0.64
1:D:132:TYR:O	1:D:134:LEU:HG	1.98	0.64
1:C:57:ARG:O	1:C:57:ARG:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:THR:O	1:D:165:GLY:N	2.31	0.63
1:B:3:LEU:CD2	1:B:19:LEU:HD13	2.30	0.62
1:C:318:ASP:OD2	1:C:322:LYS:HE3	2.00	0.61
1:A:299:PRO:HG3	1:C:317:ASP:HB3	1.83	0.61
1:D:51:LEU:HB3	1:D:84:THR:HG21	1.83	0.60
1:B:18:ARG:HD3	1:B:153:VAL:HA	1.82	0.60
1:D:93:ASP:OD1	1:D:93:ASP:C	2.43	0.60
1:C:24:HIS:CD2	1:C:152:THR:HG21	2.36	0.60
1:B:3:LEU:HG	1:B:4:GLY:O	2.01	0.60
1:C:8:LEU:HD12	1:C:30:ASP:HB2	1.82	0.60
1:A:251:ARG:NH1	1:B:160:ALA:O	2.34	0.60
1:C:247:GLU:O	1:C:250:ARG:HB2	2.02	0.60
1:A:247:GLU:OE1	1:A:251:ARG:NH2	2.35	0.59
1:D:184:GLY:O	1:D:186:GLY:N	2.36	0.59
1:A:3:LEU:CD2	1:A:19:LEU:HD13	2.32	0.59
1:A:30:ASP:O	1:A:31:HIS:C	2.46	0.58
1:A:134:LEU:HD11	1:A:153:VAL:HG22	1.85	0.58
1:B:178:LEU:HD23	1:B:180:CYS:SG	2.43	0.58
1:C:192:VAL:O	1:C:196:ILE:HG13	2.04	0.58
1:B:282:ASP:OD1	1:B:314:ARG:NH2	2.37	0.58
1:A:13:ALA:O	1:A:16:VAL:HB	2.04	0.57
1:C:283:SER:HB2	1:C:285:GLU:OE2	2.04	0.57
1:C:58:LEU:HB3	1:C:62:ARG:HG2	1.87	0.57
1:A:282:ASP:OD1	1:A:314:ARG:NH2	2.35	0.56
1:D:120:GLY:O	1:D:134:LEU:HA	2.05	0.56
1:C:122:SER:OG	1:C:123:GLY:N	2.29	0.55
1:B:329:LYS:O	1:B:330:GLN:HG2	2.06	0.55
1:B:184:GLY:O	1:B:186:GLY:N	2.40	0.55
1:A:65:TRP:CE3	1:A:92:ILE:HG21	2.42	0.55
1:A:172:PRO:O	1:A:173:SER:C	2.50	0.55
1:D:74:THR:O	1:D:78:ILE:HG12	2.07	0.55
1:C:206:GLU:CD	1:D:300:ALA:HA	2.32	0.55
1:D:173:SER:HB3	1:D:178:LEU:HD13	1.89	0.55
1:C:304:THR:O	1:C:308:GLN:HG2	2.06	0.55
1:A:3:LEU:HD12	1:A:63:VAL:HG12	1.89	0.54
1:A:301:PRO:HD2	1:B:206:GLU:OE1	2.08	0.54
1:C:139:ASP:HB3	1:C:142:ALA:HB3	1.89	0.54
1:C:81:LEU:HD22	1:C:85:LEU:HD11	1.90	0.54
1:D:13:ALA:O	1:D:16:VAL:N	2.41	0.54
1:D:103:LEU:HD23	1:D:183:CYS:SG	2.48	0.54
1:A:75:THR:HG23	1:A:105:HIS:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HA	1:B:258:TRP:CE3	2.44	0.53
1:D:146:ALA:O	1:D:149:ILE:N	2.40	0.53
1:B:109:LEU:HB3	1:B:114:ILE:HB	1.90	0.52
1:D:55:SER:O	1:D:62:ARG:NE	2.36	0.52
1:A:305:THR:HG21	1:B:301:PRO:CB	2.34	0.51
1:C:134:LEU:HD11	1:C:153:VAL:CG2	2.40	0.51
1:A:43:ASP:OD1	1:A:44:ARG:HG3	2.10	0.51
1:D:272:ASP:O	1:D:273:LEU:C	2.53	0.51
1:D:2:GLN:HA	1:D:25:ASP:O	2.09	0.51
1:B:138:GLY:H	1:B:182:PRO:C	2.18	0.51
1:C:282:ASP:OD2	1:C:314:ARG:NH2	2.38	0.51
1:B:297:GLY:O	1:D:316:LEU:HD13	2.11	0.51
1:D:157:VAL:N	1:D:175:GLN:HA	2.26	0.51
1:C:57:ARG:O	1:C:57:ARG:CG	2.58	0.51
1:D:91:VAL:O	1:D:116:LEU:HD12	2.11	0.51
1:B:51:LEU:O	1:B:54:LEU:HB3	2.11	0.50
1:C:127:GLY:O	1:C:131:GLY:CA	2.59	0.50
1:B:77:VAL:O	1:B:81:LEU:HD12	2.12	0.50
1:C:119:CYS:SG	1:C:134:LEU:HD22	2.51	0.50
1:D:106:GLU:O	1:D:110:PHE:HB2	2.11	0.50
1:A:3:LEU:HD23	1:A:19:LEU:HD13	1.95	0.49
1:C:302:VAL:CG1	1:D:302:VAL:HG13	2.40	0.49
1:A:322:LYS:HE2	1:D:276:PHE:O	2.12	0.49
1:C:190:LYS:O	1:C:193:HIS:HB3	2.13	0.49
1:B:132:TYR:O	1:B:134:LEU:HG	2.13	0.49
1:A:302:VAL:HG13	1:B:302:VAL:HG13	1.93	0.49
1:C:293:ALA:HB2	1:D:210:ILE:CD1	2.42	0.49
1:C:296:GLU:OE2	1:D:210:ILE:O	2.30	0.49
1:B:3:LEU:HD22	1:B:19:LEU:HD13	1.95	0.49
1:B:91:VAL:O	1:B:116:LEU:HD12	2.13	0.48
1:D:16:VAL:HG13	1:D:26:CYS:SG	2.53	0.48
1:D:97:THR:HG22	1:D:101:ASP:HB2	1.94	0.48
1:B:94:GLY:HA2	1:B:119:CYS:O	2.13	0.48
1:A:102:ASP:OD2	1:A:187:HIS:ND1	2.45	0.48
1:C:257:SER:HA	1:D:257:SER:HA	1.96	0.47
1:C:293:ALA:HB2	1:D:210:ILE:HD13	1.96	0.47
1:D:98:TYR:O	1:D:100:ARG:N	2.47	0.47
1:A:305:THR:HG22	1:B:302:VAL:CG2	2.43	0.47
1:D:182:PRO:O	1:D:185:SER:HB3	2.15	0.47
1:B:216:VAL:HG13	1:B:230:LEU:HD22	1.97	0.47
1:C:3:LEU:CD2	1:C:19:LEU:HD13	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:PRO:HB2	1:D:305:THR:HG23	1.95	0.47
1:D:198:TYR:CE2	1:D:286:GLY:HA3	2.50	0.47
1:C:300:ALA:HA	1:D:206:GLU:CD	2.40	0.47
1:B:198:TYR:CE2	1:B:286:GLY:HA3	2.50	0.46
1:B:234:GLU:HA	1:B:237:GLN:NE2	2.24	0.46
1:D:65:TRP:CD2	1:D:92:ILE:HG21	2.50	0.46
1:B:30:ASP:O	1:B:31:HIS:C	2.58	0.46
1:B:304:THR:O	1:B:308:GLN:CG	2.63	0.46
1:B:184:GLY:O	1:B:187:HIS:N	2.49	0.46
1:A:122:SER:OG	1:A:123:GLY:N	2.49	0.46
1:C:302:VAL:HG22	1:D:305:THR:HG22	1.97	0.46
1:A:216:VAL:HG13	1:A:230:LEU:HD22	1.96	0.46
1:B:304:THR:O	1:B:308:GLN:HG3	2.15	0.46
1:A:244:GLU:OE2	1:A:244:GLU:HA	2.15	0.45
1:D:60:ALA:HB2	1:D:62:ARG:NH1	2.32	0.45
1:B:11:MET:O	1:B:14:ASN:N	2.49	0.45
1:C:127:GLY:O	1:C:131:GLY:HA2	2.16	0.45
1:A:254:VAL:HA	1:B:258:TRP:HE3	1.81	0.45
1:C:30:ASP:OD1	1:C:31:HIS:N	2.49	0.45
1:A:291:ILE:HG23	1:C:291:ILE:HG12	1.98	0.45
1:A:206:GLU:CD	1:B:300:ALA:HA	2.41	0.45
1:D:282:ASP:OD1	1:D:314:ARG:NH2	2.50	0.45
1:A:45:THR:O	1:A:46:THR:OG1	2.32	0.44
1:A:32:ASP:O	1:A:36:VAL:HG23	2.17	0.44
1:A:73:ILE:O	1:A:76:ALA:HB3	2.18	0.44
1:A:194:ASN:O	1:A:197:GLU:HB3	2.17	0.44
1:B:65:TRP:HE1	1:B:94:GLY:HA3	1.81	0.44
1:C:9:GLY:O	1:C:10:ARG:C	2.60	0.44
1:D:3:LEU:HG	1:D:4:GLY:N	2.33	0.44
1:C:109:LEU:HD12	1:C:116:LEU:HB2	1.98	0.44
1:A:247:GLU:O	1:A:250:ARG:HG3	2.18	0.44
1:A:329:LYS:O	1:A:333:GLY:N	2.50	0.44
1:A:15:ILE:HD12	1:A:67:MET:CE	2.48	0.44
1:B:305:THR:HA	1:B:308:GLN:HG3	2.00	0.44
1:A:118:ASP:O	1:A:136:ILE:HA	2.18	0.44
1:D:3:LEU:HD22	1:D:19:LEU:HD13	2.00	0.44
1:D:250:ARG:NE	1:D:261:ASP:OD1	2.44	0.43
1:B:118:ASP:CG	1:B:184:GLY:H	2.27	0.43
1:D:78:ILE:HG21	1:D:105:HIS:HB3	2.00	0.43
1:A:242:ILE:N	1:A:243:PRO:CD	2.81	0.43
1:A:275:GLU:OE1	1:A:276:PHE:CE2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:O	1:A:308:GLN:HG3	2.18	0.43
1:C:51:LEU:O	1:C:84:THR:HG23	2.18	0.43
1:D:169:GLU:OE2	1:D:169:GLU:CA	2.54	0.43
1:A:300:ALA:HA	1:B:206:GLU:CD	2.43	0.43
1:A:315:ASP:O	1:A:318:ASP:HB2	2.18	0.43
1:B:118:ASP:CG	1:B:118:ASP:O	2.62	0.43
1:D:265:ILE:O	1:D:268:ARG:N	2.38	0.43
1:B:329:LYS:C	1:B:330:GLN:CG	2.92	0.43
1:C:254:VAL:HG12	1:D:259:LEU:HD21	2.01	0.43
1:D:188:PHE:O	1:D:191:MET:HB2	2.19	0.43
1:B:29:TYR:CE2	1:B:51:LEU:CD1	3.02	0.43
1:C:258:TRP:O	1:C:262:LEU:HG	2.19	0.43
1:D:260:LEU:O	1:D:264:ALA:N	2.51	0.43
1:A:250:ARG:NH2	1:B:161:PRO:O	2.52	0.43
1:A:208:LEU:HD22	1:A:242:ILE:CG2	2.49	0.42
1:C:31:HIS:O	1:C:33:PRO:HD3	2.19	0.42
1:A:5:MET:SD	1:A:65:TRP:HB3	2.60	0.42
1:A:75:THR:O	1:A:76:ALA:C	2.62	0.42
1:C:174:GLU:O	1:D:251:ARG:NH1	2.40	0.42
1:D:98:TYR:O	1:D:101:ASP:N	2.52	0.42
1:D:198:TYR:CE1	1:D:310:ARG:NH1	2.87	0.42
1:C:285:GLU:HA	1:C:288:TRP:CE3	2.55	0.42
1:A:45:THR:C	1:A:46:THR:OG1	2.63	0.42
1:C:17:ARG:HG3	1:C:39:MET:HE1	2.02	0.42
1:B:34:ASP:OD1	1:B:34:ASP:N	2.49	0.42
1:C:252:GLY:C	1:D:133:CYS:HB2	2.44	0.42
1:C:253:SER:O	1:D:130:ARG:NH2	2.52	0.42
1:A:48:VAL:HG23	1:A:49:ALA:N	2.34	0.42
1:C:251:ARG:NH1	1:D:160:ALA:O	2.53	0.42
1:A:305:THR:HG22	1:B:302:VAL:HG23	2.02	0.41
1:B:287:ARG:HD3	1:D:294:ILE:O	2.19	0.41
1:C:136:ILE:HD12	1:C:136:ILE:N	2.35	0.41
1:B:78:ILE:HG23	1:B:109:LEU:HD11	2.02	0.41
1:C:254:VAL:HA	1:D:258:TRP:CE3	2.55	0.41
1:D:67:MET:SD	1:D:94:GLY:O	2.79	0.41
1:D:317:ASP:OD1	1:D:317:ASP:N	2.51	0.41
1:B:278:GLY:CA	1:C:321:ASN:HB3	2.49	0.41
1:A:12:GLY:O	1:A:16:VAL:HG23	2.20	0.41
1:C:191:MET:SD	1:C:288:TRP:HB3	2.60	0.41
1:A:29:TYR:CD1	1:A:30:ASP:N	2.89	0.41
1:A:258:TRP:O	1:A:261:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:VAL:HA	1:D:258:TRP:HE3	1.86	0.41
1:D:34:ASP:OD1	1:D:34:ASP:N	2.53	0.41
1:D:135:MET:HB3	1:D:180:CYS:SG	2.61	0.41
1:A:262:LEU:HD22	1:D:330:GLN:HB3	2.02	0.41
1:B:29:TYR:HE2	1:B:51:LEU:CD1	2.34	0.41
1:B:190:LYS:O	1:B:193:HIS:HB3	2.21	0.41
1:C:206:GLU:OE1	1:D:301:PRO:HD2	2.20	0.41
1:D:98:TYR:O	1:D:99:TYR:C	2.64	0.41
1:D:263:THR:O	1:D:267:LEU:HD12	2.20	0.41
1:A:305:THR:CG2	1:B:301:PRO:CB	2.92	0.41
1:B:32:ASP:O	1:B:36:VAL:HG23	2.21	0.41
1:C:77:VAL:HG12	1:C:81:LEU:HD12	2.02	0.41
1:C:149:ILE:O	1:C:153:VAL:HG13	2.21	0.41
1:D:284:GLY:HA2	1:D:287:ARG:HG3	2.03	0.41
1:C:28:VAL:HG21	1:C:39:MET:HB2	2.03	0.40
1:C:194:ASN:HD22	1:C:285:GLU:CB	2.34	0.40
1:A:302:VAL:CG2	1:B:305:THR:HG22	2.42	0.40
1:A:184:GLY:O	1:A:185:SER:C	2.65	0.40
1:A:200:MET:HE3	1:B:200:MET:HE3	2.01	0.40
1:D:184:GLY:O	1:D:185:SER:C	2.65	0.40
1:A:243:PRO:HG2	1:A:271:PRO:HB3	2.04	0.40
1:C:127:GLY:O	1:C:131:GLY:N	2.54	0.40
1:B:329:LYS:C	1:B:329:LYS:HD3	2.47	0.40
1:C:242:ILE:N	1:C:243:PRO:CD	2.83	0.40
1:D:77:VAL:HG12	1:D:81:LEU:HD12	2.03	0.40
1:D:320:ALA:O	1:D:323:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

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	329/340 (97%)	291 (88%)	29 (9%)	9 (3%)	4	6
1	B	319/340 (94%)	273 (86%)	45 (14%)	1 (0%)	36	54
1	C	327/340 (96%)	294 (90%)	32 (10%)	1 (0%)	36	54
1	D	321/340 (94%)	267 (83%)	40 (12%)	14 (4%)	2	2
All	All	1296/1360 (95%)	1125 (87%)	146 (11%)	25 (2%)	6	10

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	SER
1	C	84	THR
1	D	185	SER
1	A	31	HIS
1	A	46	THR
1	A	49	ALA
1	A	273	LEU
1	D	43	ASP
1	D	99	TYR
1	D	164	PRO
1	A	29	TYR
1	D	269	GLU
1	A	166	ARG
1	D	23	GLY
1	D	176	GLY
1	D	182	PRO
1	D	172	PRO
1	A	16	VAL
1	A	333	GLY
1	D	265	ILE
1	A	48	VAL
1	D	125	VAL
1	D	12	GLY
1	D	195	GLY
1	D	161	PRO

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	254/259 (98%)	237 (93%)	17 (7%)	15	27
1	B	248/259 (96%)	228 (92%)	20 (8%)	11	20
1	C	253/259 (98%)	232 (92%)	21 (8%)	10	19
1	D	250/259 (96%)	218 (87%)	32 (13%)	4	7
All	All	1005/1036 (97%)	915 (91%)	90 (9%)	9	17

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	36	VAL
1	A	44	ARG
1	A	45	THR
1	A	50	SER
1	A	51	LEU
1	A	55	SER
1	A	59	SER
1	A	106	GLU
1	A	153	VAL
1	A	193	HIS
1	A	216	VAL
1	A	227	THR
1	A	251	ARG
1	A	283	SER
1	A	305	THR
1	A	328	ARG
1	B	34	ASP
1	B	36	VAL
1	B	45	THR
1	B	48	VAL
1	B	52	ARG
1	B	58	LEU
1	B	110	PHE
1	B	157	VAL
1	B	163	THR
1	B	178	LEU
1	B	185	SER
1	B	204	LEU
1	B	216	VAL
1	B	243	PRO

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Mol	Chain	Res	Type
1	B	251	ARG
1	B	253	SER
1	B	285	GLU
1	B	305	THR
1	B	325	SER
1	B	329	LYS
1	C	10	ARG
1	C	27	VAL
1	C	37	LYS
1	C	45	THR
1	C	51	LEU
1	C	58	LEU
1	C	80	GLU
1	C	84	THR
1	C	108	LEU
1	C	110	PHE
1	C	114	ILE
1	C	121	THR
1	C	141	ASP
1	C	152	THR
1	C	153	VAL
1	C	219	ARG
1	C	220	VAL
1	C	237	GLN
1	C	251	ARG
1	C	254	VAL
1	C	305	THR
1	D	1	MET
1	D	11	MET
1	D	34	ASP
1	D	46	THR
1	D	59	SER
1	D	72	ASN
1	D	84	THR
1	D	86	GLU
1	D	107	LYS
1	D	108	LEU
1	D	110	PHE
1	D	112	LYS
1	D	114	ILE
1	D	118	ASP
1	D	121	THR

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Mol	Chain	Res	Type
1	D	129	GLU
1	D	134	LEU
1	D	135	MET
1	D	152	THR
1	D	163	THR
1	D	169	GLU
1	D	172	PRO
1	D	185	SER
1	D	204	LEU
1	D	227	THR
1	D	248	VAL
1	D	251	ARG
1	D	279	ARG
1	D	282	ASP
1	D	283	SER
1	D	305	THR
1	D	325	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	237	GLN
1	B	232	ASN
1	B	237	GLN
1	C	334	HIS
1	D	72	ASN
1	D	105	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/340 (97%)	-0.01	6 (1%) 67 64	30, 67, 129, 165	0
1	B	323/340 (95%)	0.06	5 (1%) 72 69	28, 68, 138, 174	0
1	C	331/340 (97%)	0.08	2 (0%) 85 85	29, 74, 121, 165	0
1	D	325/340 (95%)	0.40	25 (7%) 19 19	32, 81, 172, 243	0
All	All	1312/1360 (96%)	0.13	38 (2%) 53 51	28, 72, 143, 243	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	54	LEU	4.5
1	D	36	VAL	4.3
1	D	51	LEU	3.8
1	D	110	PHE	3.7
1	D	39	MET	3.6
1	B	331	PHE	3.5
1	D	27	VAL	3.4
1	C	126	TRP	3.3
1	A	126	TRP	3.1
1	D	2	GLN	3.0
1	D	47	GLY	3.0
1	D	38	ALA	3.0
1	D	3	LEU	2.8
1	A	339	ALA	2.7
1	D	117	LEU	2.7
1	D	220	VAL	2.6
1	A	39	MET	2.6
1	A	49	ALA	2.6
1	D	28	VAL	2.6
1	B	63	VAL	2.5
1	D	40	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	130	ARG	2.4
1	D	63	VAL	2.4
1	D	29	TYR	2.3
1	B	54	LEU	2.3
1	D	170	VAL	2.3
1	D	35	ALA	2.3
1	D	61	PRO	2.3
1	D	60	ALA	2.2
1	D	33	PRO	2.1
1	A	54	LEU	2.1
1	D	24	HIS	2.1
1	A	48	VAL	2.1
1	D	55	SER	2.1
1	D	229	PRO	2.0
1	B	110	PHE	2.0
1	B	50	SER	2.0
1	D	90	ILE	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.