



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:25 PM UTC

PDB ID : 3WAD / pdb_00003wad
Title : Crystal structure of glycosyltransferase VinC involved in the biosynthesis of vicienistatin
Authors : Nango, E.; Minami, A.; Kumasaka, T.; Eguchi, T.
Deposited on : 2013-05-02
Resolution : 2.00 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

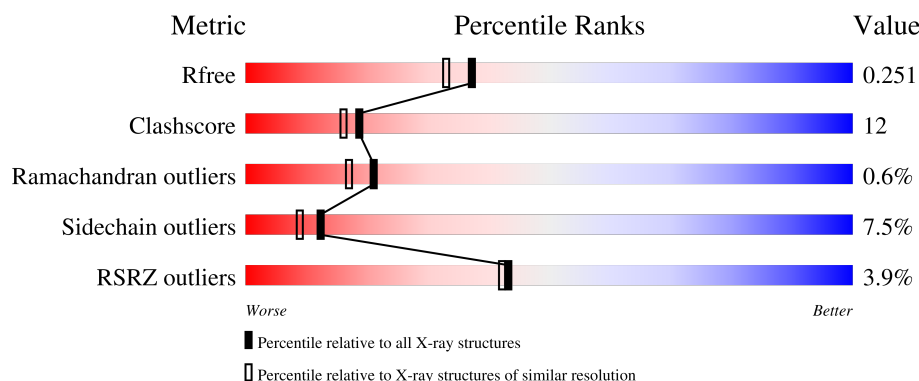
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	419	 4% 67% 24% 5%
1	B	419	 3% 68% 23% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6639 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	1	0
			3101	1968	544	577	12			
1	B	401	Total	C	N	O	S	0	0	0
			3116	1975	550	579	12			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

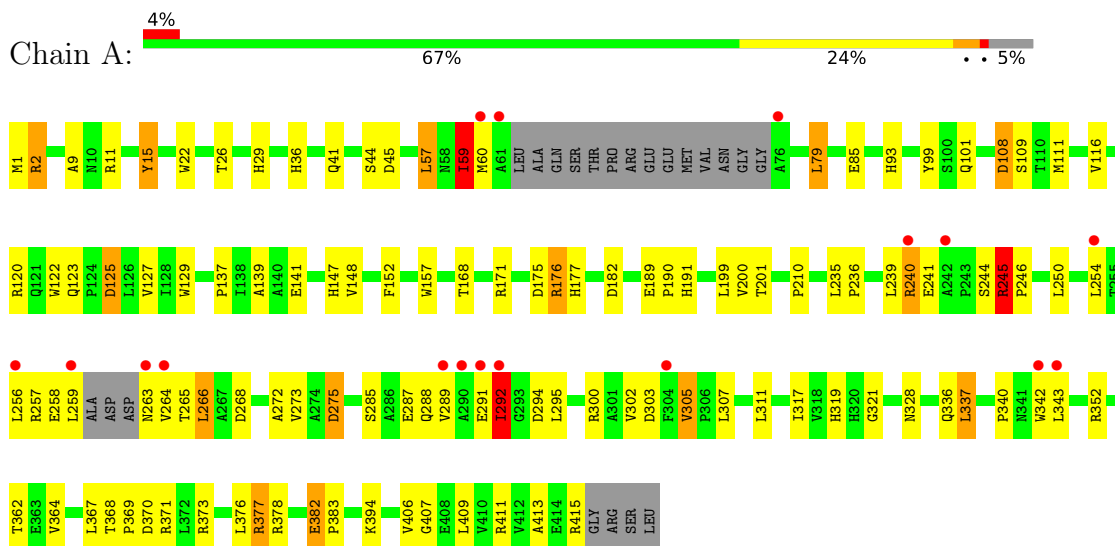
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	207	Total	O	0	0
			207	207		
3	B	214	Total	O	0	0
			214	214		

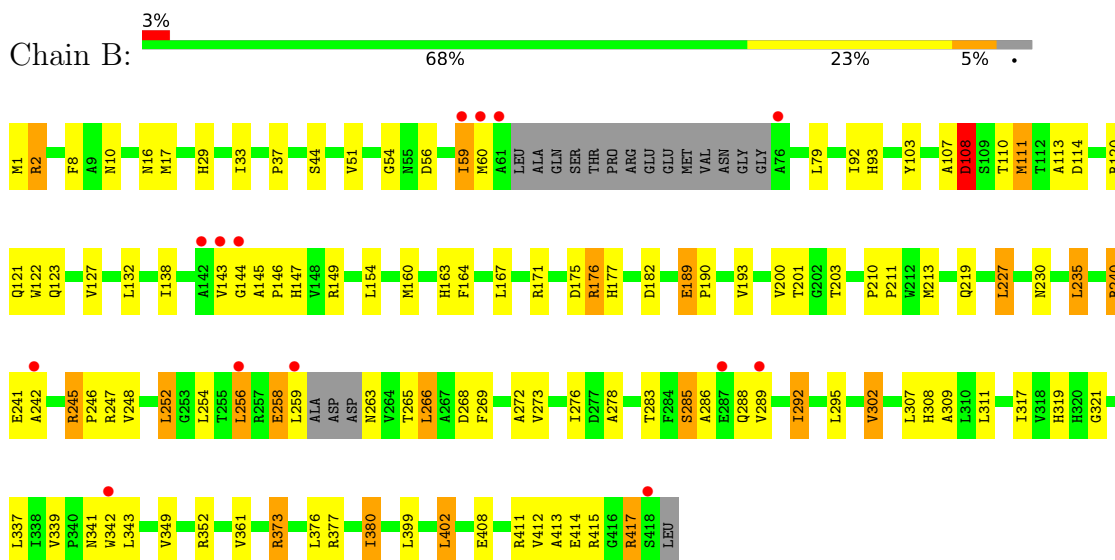
3 Residue-property plots [i](#)

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: Glycosyltransferase



- Molecule 1: Glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.20Å 130.39Å 140.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.21 – 2.00 40.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.21-2.00) 98.6 (40.21-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.202 , 0.253 0.203 , 0.251	Depositor DCC
R_{free} test set	3100 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6639	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.33	9/3183 (0.3%)	1.26	22/4358 (0.5%)
1	B	1.41	20/3195 (0.6%)	1.26	18/4373 (0.4%)
All	All	1.37	29/6378 (0.5%)	1.26	40/8731 (0.5%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	LEU	CA-C	7.76	1.61	1.52
1	B	33	ILE	CA-CB	6.66	1.62	1.53
1	A	292	ILE	CA-CB	6.51	1.62	1.54
1	B	113	ALA	C-O	6.44	1.31	1.24
1	B	146	PRO	CA-C	6.33	1.60	1.52
1	B	143	VAL	CA-CB	6.17	1.62	1.54
1	B	17	MET	SD-CE	-6.12	1.64	1.79
1	B	138	ILE	C-O	6.10	1.31	1.24
1	B	203	THR	CA-C	-6.07	1.44	1.52
1	B	59	ILE	CA-CB	6.00	1.62	1.54
1	B	412	VAL	CA-CB	5.93	1.61	1.54
1	B	193	VAL	C-O	5.72	1.30	1.24
1	A	364	VAL	CA-CB	5.65	1.56	1.54
1	B	108	ASP	CB-CG	-5.61	1.38	1.52
1	A	342	TRP	CA-C	5.60	1.60	1.53
1	A	352	ARG	N-CA	5.56	1.52	1.46
1	A	108	ASP	CB-CG	-5.34	1.38	1.52
1	B	380	ILE	CA-CB	5.34	1.61	1.54
1	A	125	ASP	C-O	5.33	1.30	1.24
1	B	309	ALA	N-CA	5.31	1.53	1.46
1	A	406	VAL	CA-CB	5.28	1.61	1.54
1	B	373	ARG	C-O	5.27	1.30	1.24
1	A	210	PRO	N-CA	5.21	1.52	1.46
1	B	16	ASN	CA-C	5.11	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	VAL	CA-CB	5.10	1.60	1.54
1	B	143	VAL	C-O	5.09	1.30	1.24
1	A	407	GLY	N-CA	5.09	1.52	1.45
1	B	51	VAL	CA-CB	5.05	1.58	1.54
1	B	144	GLY	C-O	5.04	1.29	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	MET	CG-SD-CE	-9.16	80.74	100.90
1	A	59	ILE	CB-CA-C	-8.37	99.18	112.16
1	B	399	LEU	CA-C-N	-7.49	112.04	119.90
1	B	399	LEU	C-N-CA	-7.49	112.04	119.90
1	A	108	ASP	N-CA-C	7.01	125.73	110.80
1	A	305	VAL	CA-C-N	-6.76	112.80	119.90
1	A	305	VAL	C-N-CA	-6.76	112.80	119.90
1	B	108	ASP	CB-CG-OD1	-6.73	102.92	118.40
1	A	123	GLN	CA-C-N	-6.47	113.09	119.76
1	A	123	GLN	C-N-CA	-6.47	113.09	119.76
1	B	203	THR	N-CA-C	-6.31	103.70	111.33
1	A	157	TRP	CA-C-N	6.30	127.11	119.99
1	A	157	TRP	C-N-CA	6.30	127.11	119.99
1	B	219	GLN	CA-C-N	-6.25	114.19	120.31
1	B	219	GLN	C-N-CA	-6.25	114.19	120.31
1	B	44	SER	N-CA-C	5.93	117.74	111.28
1	A	152	PHE	N-CA-C	-5.90	104.56	113.89
1	A	317	ILE	N-CA-C	5.73	116.14	108.11
1	B	258	GLU	N-CA-C	5.73	119.37	112.38
1	B	145	ALA	CA-C-N	5.70	125.66	119.78
1	B	145	ALA	C-N-CA	5.70	125.66	119.78
1	B	108	ASP	CA-CB-CG	-5.69	106.91	112.60
1	A	15	TYR	CA-C-N	5.62	128.08	120.38
1	A	15	TYR	C-N-CA	5.62	128.08	120.38
1	A	340	PRO	CA-C-N	5.61	127.80	120.28
1	A	340	PRO	C-N-CA	5.61	127.80	120.28
1	B	189	GLU	CA-C-N	-5.34	114.31	119.87
1	B	189	GLU	C-N-CA	-5.34	114.31	119.87
1	B	108	ASP	N-CA-C	5.31	122.12	110.80
1	B	412	VAL	CB-CA-C	-5.30	105.08	112.02
1	A	303	ASP	CB-CA-C	-5.25	102.64	110.88
1	A	57	LEU	N-CA-C	-5.22	106.59	113.12
1	A	337	LEU	N-CA-C	-5.22	100.01	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ALA	CA-C-N	5.18	131.43	121.54
1	B	107	ALA	C-N-CA	5.18	131.43	121.54
1	A	22	TRP	N-CA-C	5.13	117.77	111.82
1	A	99	TYR	N-CA-C	5.11	117.74	111.82
1	A	108	ASP	CB-CG-OD1	-5.09	106.69	118.40
1	A	382	GLU	CA-C-N	5.05	124.71	119.56
1	A	382	GLU	C-N-CA	5.05	124.71	119.56

There are no chirality outliers.

There are no planarity outliers.

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	3101	0	3032	73	0
1	B	3116	0	3047	76	0
2	A	1	0	0	0	0
3	A	207	0	0	6	0
3	B	214	0	0	3	0
All	All	6639	0	6079	146	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 12.

All (146) 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:A:1:MET:HE1	1:A:413:ALA:CB	1.85	1.06
1:B:266:LEU:HG	1:B:292:ILE:HG22	1.38	1.05
1:B:373:ARG:HD2	1:B:377:ARG:HH21	1.29	0.98
1:B:265:THR:HG22	1:B:268:ASP:CG	1.92	0.95
1:B:288:GLN:O	1:B:292:ILE:HG23	1.65	0.95
1:B:341:ASN:HD22	1:B:342:TRP:H	0.98	0.94
1:B:292:ILE:HD11	1:B:295:LEU:HD23	1.50	0.93
1:B:341:ASN:ND2	1:B:342:TRP:H	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HD22	1:B:342:TRP:N	1.69	0.89
1:A:288:GLN:O	1:A:292:ILE:HG23	1.75	0.85
1:A:1:MET:HE1	1:A:413:ALA:HB1	1.61	0.83
1:B:230:ASN:HD22	1:B:308:HIS:HD2	1.27	0.81
1:A:373:ARG:HG2	1:A:377:ARG:HH12	1.47	0.78
1:A:378:ARG:HG2	1:A:382:GLU:OE1	1.84	0.78
1:A:373:ARG:HG2	1:A:377:ARG:NH1	1.99	0.77
1:A:275:ASP:HB3	1:A:373:ARG:HD2	1.67	0.76
1:B:93:HIS:NE2	1:B:177:HIS:HD2	1.83	0.76
1:A:272:ALA:O	1:A:373:ARG:HG3	1.84	0.76
1:A:189:GLU:HG3	1:A:190:PRO:HD3	1.69	0.75
1:A:141:GLU:HG3	1:A:199:LEU:HD21	1.69	0.74
1:B:265:THR:HG23	1:B:268:ASP:H	1.53	0.72
1:B:200:VAL:HG12	1:B:201:THR:HG23	1.71	0.72
1:B:213:MET:HE3	1:B:349:VAL:HG22	1.71	0.72
1:B:120:ARG:O	1:B:123:GLN:HG2	1.91	0.71
1:B:240:ARG:HH11	1:B:240:ARG:HG2	1.55	0.71
1:A:370:ASP:OD1	1:A:373:ARG:NH1	2.24	0.70
1:A:287:GLU:O	1:A:291:GLU:HG3	1.91	0.70
1:B:373:ARG:CD	1:B:377:ARG:HH21	2.04	0.70
1:A:93:HIS:NE2	1:A:177:HIS:HD2	1.90	0.69
1:B:240:ARG:HH11	1:B:240:ARG:CG	2.06	0.68
1:B:265:THR:CG2	1:B:268:ASP:H	2.09	0.66
1:B:285:SER:HB2	1:B:288:GLN:H	1.60	0.66
1:A:319:HIS:HE1	1:A:336:GLN:OE1	1.80	0.64
1:B:1:MET:HE1	1:B:413:ALA:CB	2.27	0.64
1:B:154:LEU:HD21	1:B:213:MET:CE	2.28	0.64
1:B:177:HIS:HE1	1:B:182:ASP:OD2	1.80	0.64
1:B:266:LEU:HG	1:B:292:ILE:CG2	2.22	0.62
1:B:245:ARG:HB2	1:B:246:PRO:CD	2.30	0.62
1:A:168:THR:O	1:A:176:ARG:HD2	2.00	0.62
1:A:191:HIS:HE1	3:A:702:HOH:O	1.81	0.62
1:B:230:ASN:HD22	1:B:308:HIS:CD2	2.12	0.61
1:A:285:SER:O	1:A:289:VAL:HG23	2.00	0.61
1:A:287:GLU:H	1:A:287:GLU:CD	2.09	0.60
1:A:177:HIS:HE1	1:A:182:ASP:OD2	1.84	0.59
1:B:373:ARG:HD2	1:B:377:ARG:NH2	2.11	0.59
1:A:177:HIS:CE1	1:A:182:ASP:OD2	2.57	0.58
1:B:175:ASP:C	1:B:176:ARG:HG2	2.29	0.58
1:B:252:LEU:HD11	1:B:339:VAL:HG21	1.86	0.58
1:A:1:MET:HG2	1:A:29:HIS:ND1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:HIS:CD2	1:B:321:GLY:H	2.23	0.57
1:B:411:ARG:HB3	1:B:415:ARG:NH1	2.20	0.57
1:A:319:HIS:CD2	1:A:321:GLY:H	2.24	0.56
1:B:154:LEU:HD21	1:B:213:MET:HE2	1.87	0.56
1:A:244:SER:O	1:A:245:ARG:HB3	2.04	0.56
1:A:85[B]:GLU:CD	1:A:85[B]:GLU:H	2.14	0.55
1:A:141:GLU:HG3	1:A:199:LEU:CD2	2.35	0.55
1:B:213:MET:CE	1:B:349:VAL:HG22	2.35	0.55
1:A:240:ARG:O	1:B:121:GLN:HG3	2.06	0.55
1:A:373:ARG:CG	1:A:377:ARG:HH12	2.16	0.54
1:B:235:LEU:HD23	1:B:240:ARG:HG3	1.88	0.54
1:B:245:ARG:HB2	1:B:246:PRO:HD2	1.89	0.53
1:A:373:ARG:NE	1:A:377:ARG:HH12	2.07	0.53
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.75	0.52
1:A:319:HIS:CE1	1:A:336:GLN:OE1	2.61	0.52
1:A:116:VAL:HG22	1:A:139:ALA:HA	1.91	0.52
1:A:241:GLU:N	1:A:241:GLU:OE1	2.43	0.52
1:A:285:SER:OG	1:A:288:GLN:HG3	2.09	0.52
1:A:259:LEU:HD23	1:A:367:LEU:HD23	1.92	0.51
1:A:265:THR:O	1:A:268:ASP:HB2	2.09	0.51
1:A:1:MET:HE1	1:A:413:ALA:HB2	1.84	0.51
1:A:9:ALA:HB2	1:A:36:HIS:HB2	1.91	0.51
1:B:1:MET:HG2	1:B:29:HIS:ND1	2.24	0.51
1:B:408:GLU:CD	1:B:411:ARG:HH12	2.18	0.50
1:B:177:HIS:CE1	1:B:182:ASP:OD2	2.61	0.50
1:B:2:ARG:HD2	1:B:122:TRP:CE2	2.47	0.49
1:B:92:ILE:HG21	1:B:164:PHE:HB2	1.94	0.49
1:A:57:LEU:HD21	1:A:59:ILE:HG23	1.95	0.49
1:A:295:LEU:HD13	3:A:759:HOH:O	2.12	0.49
1:A:148:VAL:HG21	1:A:409:LEU:CD2	2.43	0.48
1:B:240:ARG:HG2	1:B:240:ARG:NH1	2.22	0.48
1:A:200:VAL:HG12	1:A:201:THR:HG23	1.94	0.48
1:B:411:ARG:O	1:B:415:ARG:HB2	2.14	0.48
1:B:93:HIS:NE2	1:B:177:HIS:CD2	2.74	0.48
1:B:286:ALA:O	1:B:289:VAL:HG12	2.13	0.48
1:B:103:TYR:CZ	1:B:132:LEU:HD22	2.50	0.47
1:A:311:LEU:HD12	1:A:328:ASN:HB3	1.96	0.47
1:A:101:GLN:HG2	3:A:751:HOH:O	2.14	0.47
1:A:109:SER:HA	3:A:700:HOH:O	2.15	0.47
1:A:79:LEU:HB3	3:A:767:HOH:O	2.14	0.46
1:A:127:VAL:O	1:A:147:HIS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:TRP:CD2	1:A:137:PRO:HD3	2.50	0.46
1:A:263:ASN:ND2	1:A:264:VAL:HG13	2.30	0.46
1:A:373:ARG:HE	1:A:377:ARG:HH22	1.62	0.46
1:A:250:LEU:HD22	1:A:273:VAL:HG11	1.96	0.46
1:A:171:ARG:O	1:A:176:ARG:NH1	2.38	0.46
1:A:171:ARG:HD3	1:A:175:ASP:O	2.16	0.46
1:A:368:THR:O	1:A:369:PRO:C	2.58	0.46
1:A:245:ARG:O	1:A:246:PRO:C	2.59	0.45
1:A:240:ARG:NH2	1:B:114:ASP:O	2.49	0.45
1:B:8:PHE:CE1	1:B:10:ASN:HB2	2.51	0.45
1:B:272:ALA:O	1:B:373:ARG:HG3	2.16	0.45
1:B:341:ASN:CG	1:B:343:LEU:HD13	2.41	0.45
1:B:154:LEU:HD21	1:B:213:MET:HE3	1.97	0.44
1:B:240:ARG:HH11	1:B:240:ARG:CB	2.29	0.44
1:B:248:VAL:HG11	1:B:376:LEU:HD21	1.99	0.44
1:A:373:ARG:CD	1:A:377:ARG:HH12	2.31	0.44
1:B:341:ASN:ND2	1:B:342:TRP:N	2.46	0.44
1:A:362:THR:OG1	1:A:371:ARG:HD3	2.17	0.44
1:B:127:VAL:O	1:B:147:HIS:HA	2.17	0.44
1:B:79:LEU:HD12	1:B:160:MET:HG3	1.99	0.44
1:A:11:ARG:HD3	1:A:15:TYR:OH	2.18	0.43
1:B:241:GLU:O	1:B:242:ALA:C	2.61	0.43
1:B:269:PHE:O	1:B:273:VAL:HG23	2.18	0.43
1:A:266:LEU:HB3	1:A:292:ILE:HG22	1.99	0.43
1:A:377:ARG:CG	1:A:377:ARG:HH11	2.31	0.43
1:B:54:GLY:HA2	1:B:110:THR:HG22	2.00	0.43
1:A:93:HIS:NE2	1:A:177:HIS:CD2	2.80	0.43
1:B:240:ARG:CG	1:B:240:ARG:NH1	2.75	0.42
1:B:213:MET:CE	1:B:349:VAL:CG2	2.97	0.42
1:A:411:ARG:O	1:A:415:ARG:HG2	2.20	0.42
1:A:373:ARG:HE	1:A:377:ARG:HH12	1.68	0.42
1:B:189:GLU:HB3	1:B:190:PRO:HD3	2.00	0.42
1:B:240:ARG:HH11	1:B:240:ARG:HB3	1.84	0.42
1:B:283:THR:HA	1:B:302:VAL:O	2.20	0.42
1:B:210:PRO:HA	1:B:211:PRO:HD3	1.91	0.42
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.84	0.42
1:B:414:GLU:HA	1:B:417:ARG:HD2	2.02	0.42
1:A:382:GLU:HA	1:A:383:PRO:HD2	1.88	0.41
1:B:108:ASP:HB3	1:B:111:MET:H	1.84	0.41
1:A:236:PRO:HD2	1:A:239:LEU:HD12	2.02	0.41
1:B:37:PRO:HB2	1:B:56:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HD11	1:A:295:LEU:HD23	2.01	0.41
1:A:295:LEU:CD1	3:A:759:HOH:O	2.69	0.41
1:B:163:HIS:O	1:B:167:LEU:HG	2.21	0.41
1:B:227:LEU:HD21	3:B:605:HOH:O	2.20	0.41
1:B:149:ARG:HD2	3:B:699:HOH:O	2.20	0.41
1:B:123:GLN:HB3	3:B:693:HOH:O	2.20	0.41
1:A:285:SER:HB2	1:A:287:GLU:OE1	2.20	0.41
1:A:2:ARG:HB3	1:A:122:TRP:CZ2	2.56	0.41
1:B:311:LEU:HD21	1:B:317:ILE:HD12	2.03	0.40
1:A:41:GLN:NE2	1:A:45:ASP:OD1	2.54	0.40
1:A:1:MET:HE2	1:A:125:ASP:HB2	2.03	0.40
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.92	0.40
1:B:171:ARG:O	1:B:176:ARG:NH1	2.54	0.40
1:B:276:ILE:HD12	1:B:278:ALA:HB3	2.02	0.40
1:A:26:THR:HB	1:B:402:LEU:HD23	2.02	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	393/419 (94%)	378 (96%)	12 (3%)	3 (1%)	16	11
1	B	395/419 (94%)	373 (94%)	20 (5%)	2 (0%)	24	21
All	All	788/838 (94%)	751 (95%)	32 (4%)	5 (1%)	21	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	A	245	ARG
1	B	285	SER

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Mol	Chain	Res	Type
1	A	275	ASP
1	B	108	ASP

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	325/340 (96%)	300 (92%)	25 (8%)	12	8
1	B	326/340 (96%)	302 (93%)	24 (7%)	13	9
All	All	651/680 (96%)	602 (92%)	49 (8%)	12	9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	44	SER
1	A	59	ILE
1	A	60	MET
1	A	79	LEU
1	A	111	MET
1	A	176	ARG
1	A	235	LEU
1	A	240	ARG
1	A	245	ARG
1	A	254	LEU
1	A	256	LEU
1	A	257	ARG
1	A	258	GLU
1	A	266	LEU
1	A	292	ILE
1	A	294	ASP
1	A	300	ARG
1	A	302	VAL
1	A	305	VAL
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	337	LEU
1	A	343	LEU
1	A	377	ARG
1	A	394	LYS
1	B	2	ARG
1	B	59	ILE
1	B	60	MET
1	B	111	MET
1	B	176	ARG
1	B	235	LEU
1	B	240	ARG
1	B	245	ARG
1	B	247	ARG
1	B	252	LEU
1	B	254	LEU
1	B	256	LEU
1	B	258	GLU
1	B	259	LEU
1	B	263	ASN
1	B	266	LEU
1	B	292	ILE
1	B	302	VAL
1	B	307	LEU
1	B	337	LEU
1	B	352	ARG
1	B	380	ILE
1	B	402	LEU
1	B	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	121	GLN
1	A	177	HIS
1	A	191	HIS
1	A	263	ASN
1	A	308	HIS
1	A	319	HIS
1	A	320	HIS
1	A	336	GLN
1	A	341	ASN

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Mol	Chain	Res	Type
1	B	58	ASN
1	B	101	GLN
1	B	177	HIS
1	B	191	HIS
1	B	230	ASN
1	B	271	ASN
1	B	308	HIS
1	B	319	HIS
1	B	328	ASN
1	B	341	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	398/419 (94%)	0.09	17 (4%) 40 39	19, 32, 61, 75	1 (0%)
1	B	401/419 (95%)	0.05	14 (3%) 47 46	20, 31, 60, 83	0
All	All	799/838 (95%)	0.07	31 (3%) 43 42	19, 32, 61, 83	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	PHE	3.4
1	B	259	LEU	3.3
1	A	256	LEU	2.9
1	A	342	TRP	2.9
1	B	418	SER	2.9
1	A	240	ARG	2.7
1	A	259	LEU	2.7
1	B	289	VAL	2.7
1	A	61	ALA	2.6
1	B	342	TRP	2.6
1	B	61	ALA	2.5
1	B	142	ALA	2.5
1	B	76	ALA	2.5
1	B	256	LEU	2.5
1	A	292	ILE	2.5
1	B	60	MET	2.4
1	B	242	ALA	2.3
1	B	287	GLU	2.3
1	A	264	VAL	2.3
1	A	60	MET	2.3
1	A	343	LEU	2.3
1	B	59	ILE	2.2
1	A	290	ALA	2.2
1	A	263	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	289	VAL	2.1
1	B	143	VAL	2.1
1	A	242	ALA	2.1
1	A	291	GLU	2.1
1	A	254	LEU	2.0
1	B	144	GLY	2.0
1	A	76	ALA	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	500	1/1	0.81	0.38	48,48,48,48	1

6.5 Other polymers [i](#)

There are no such residues in this entry.