



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:58 AM UTC

PDB ID : 1O6C / pdb_00001o6c
Title : Crystal structure of UDP-N-acetylglucosamine 2-epimerase
Authors : Structural GenomiX
Deposited on : 2003-11-03
Resolution : 2.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

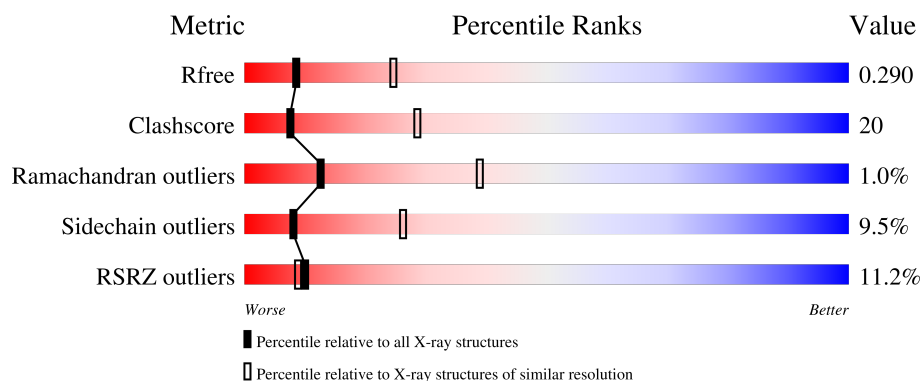
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	388	18% 55% 32% • • 8%
1	B	388	3% 55% 35% 5% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5507 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 UDP-N-acetylglucosamine 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	Se	0	0	0
			2635	1672	458	499	6			
1	B	371	Total	C	N	O	Se	0	0	0
			2860	1819	490	541	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP P39131
A	7	MSE	MET	modified residue	UNP P39131
A	19	MSE	MET	modified residue	UNP P39131
A	45	MSE	MET	modified residue	UNP P39131
A	64	MSE	MET	modified residue	UNP P39131
A	140	MSE	MET	modified residue	UNP P39131
A	201	MSE	MET	modified residue	UNP P39131
A	216	MSE	MET	modified residue	UNP P39131
A	219	MSE	MET	modified residue	UNP P39131
A	343	MSE	MET	modified residue	UNP P39131
A	381	GLY	-	cloning artifact	UNP P39131
A	382	SER	-	cloning artifact	UNP P39131
A	383	HIS	-	cloning artifact	UNP P39131
A	384	HIS	-	cloning artifact	UNP P39131
A	385	HIS	-	cloning artifact	UNP P39131
A	386	HIS	-	cloning artifact	UNP P39131
A	387	HIS	-	cloning artifact	UNP P39131
A	388	HIS	-	cloning artifact	UNP P39131
B	1	MSE	-	cloning artifact	UNP P39131
B	7	MSE	MET	modified residue	UNP P39131
B	19	MSE	MET	modified residue	UNP P39131
B	45	MSE	MET	modified residue	UNP P39131
B	64	MSE	MET	modified residue	UNP P39131
B	140	MSE	MET	modified residue	UNP P39131
B	201	MSE	MET	modified residue	UNP P39131

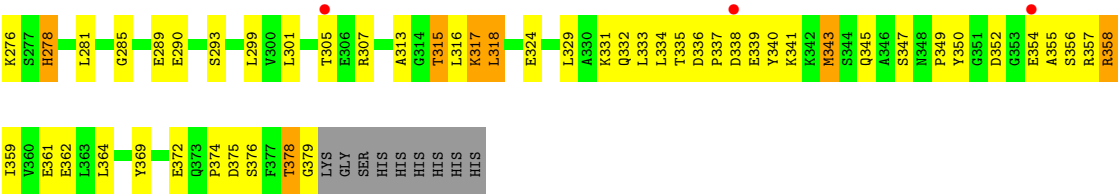
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Chain	Residue	Modelled	Actual	Comment	Reference
B	216	MSE	MET	modified residue	UNP P39131
B	219	MSE	MET	modified residue	UNP P39131
B	343	MSE	MET	modified residue	UNP P39131
B	381	GLY	-	cloning artifact	UNP P39131
B	382	SER	-	cloning artifact	UNP P39131
B	383	HIS	-	cloning artifact	UNP P39131
B	384	HIS	-	cloning artifact	UNP P39131
B	385	HIS	-	cloning artifact	UNP P39131
B	386	HIS	-	cloning artifact	UNP P39131
B	387	HIS	-	cloning artifact	UNP P39131
B	388	HIS	-	cloning artifact	UNP P39131

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	9	Total O 9 9	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.82Å 63.82Å 452.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 2.90 48.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.71-2.90) 99.3 (48.71-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.91Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.274 , 0.334 0.236 , 0.290	Depositor DCC
R_{free} test set	2141 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.3	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	0.90	EDS
Total number of atoms	5507	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	0.72	1/2673 (0.0%)	1.35	12/3606 (0.3%)
1	B	0.86	0/2908	1.49	20/3927 (0.5%)
All	All	0.79	1/5581 (0.0%)	1.42	32/7533 (0.4%)

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	A	352	ASP	CA-CB	-5.64	1.45	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ASP	CA-CB-CG	11.46	124.06	112.60
1	A	173	GLY	N-CA-C	-8.97	101.63	112.48
1	B	174	ASN	CA-CB-CG	8.27	120.87	112.60
1	B	173	GLY	N-CA-C	-7.06	103.94	112.48
1	B	97	GLY	N-CA-C	6.80	123.72	111.34
1	B	124	ARG	CD-NE-CZ	-6.48	115.33	124.40
1	A	88	ILE	N-CA-C	6.29	116.44	110.53
1	B	239	VAL	CB-CA-C	-6.04	101.37	110.55
1	B	80	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	B	174	ASN	OD1-CG-ND2	-5.95	116.66	122.60
1	B	146	ASP	N-CA-C	-5.94	106.58	113.88
1	B	173	GLY	CA-C-O	-5.93	117.08	122.24
1	B	261	LEU	CA-C-O	-5.64	113.95	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	GLY	N-CA-C	5.57	123.13	115.27
1	A	370	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	B	98	ASP	N-CA-C	5.55	119.22	111.56
1	A	352	ASP	CB-CA-C	5.48	119.89	111.02
1	A	173	GLY	CA-C-O	-5.47	117.48	122.24
1	B	278	HIS	N-CA-C	-5.32	104.38	112.04
1	B	122	GLY	N-CA-C	5.31	122.42	115.36
1	A	166	ALA	CA-C-N	5.30	131.66	121.54
1	A	166	ALA	C-N-CA	5.30	131.66	121.54
1	B	358	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	B	357	ARG	CD-NE-CZ	5.23	131.72	124.40
1	B	225	ARG	CD-NE-CZ	5.16	131.63	124.40
1	A	370	ARG	CD-NE-CZ	-5.14	117.21	124.40
1	B	222	ALA	O-C-N	5.10	127.39	122.09
1	B	42	HIS	CA-C-N	5.09	127.81	120.38
1	B	42	HIS	C-N-CA	5.09	127.81	120.38
1	B	32	ILE	N-CA-C	5.08	115.90	108.53
1	A	172	THR	N-CA-CB	-5.05	103.07	110.40
1	A	97	GLY	N-CA-C	5.04	120.39	111.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	ASP	Mainchain

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	2635	0	2488	107	0
1	B	2860	0	2807	119	0
2	A	3	0	0	0	0
2	B	9	0	0	2	0
All	All	5507	0	5295	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 20.

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:B:305:THR:HB	1:B:318:LEU:HD11	1.34	1.04
1:A:43:ARG:HH21	1:A:57:PRO:HG2	1.26	0.98
1:B:333:LEU:HD21	1:B:343:MSE:HE3	1.47	0.95
1:B:39:THR:HB	1:B:63:ILE:HD12	1.51	0.93
1:B:204:LEU:HD11	1:B:219:MSE:SE	2.22	0.90
1:A:136:LEU:HD21	1:B:144:ILE:HG12	1.53	0.90
1:A:98:ASP:HB3	1:A:138:ARG:HG3	1.56	0.85
1:A:223:ILE:HA	1:A:226:ILE:HD12	1.60	0.82
1:B:361:GLU:HB2	1:B:374:PRO:HG3	1.61	0.82
1:A:98:ASP:OD2	1:A:134:GLU:HB3	1.80	0.82
1:B:8:THR:HG22	1:B:19:MSE:HE3	1.62	0.81
1:B:315:THR:HG22	1:B:316:LEU:HG	1.64	0.78
1:B:123:LEU:O	1:B:138:ARG:HD3	1.83	0.78
1:B:1:MSE:HE3	1:B:31:GLU:OE1	1.84	0.77
1:A:39:THR:HG23	1:A:63:ILE:CD1	2.15	0.77
1:B:125:THR:HG21	1:B:130:SER:O	1.86	0.75
1:B:203:LEU:HD21	1:B:270:PHE:CE1	2.21	0.75
1:A:131:PRO:HG2	1:A:134:GLU:HB2	1.70	0.74
1:A:8:THR:HG23	1:A:19:MSE:HE3	1.72	0.72
1:B:341:LYS:HE3	1:B:345:GLN:HE22	1.52	0.72
1:B:125:THR:HG22	1:B:127:ASN:H	1.55	0.72
1:A:146:ASP:OD2	1:B:128:LYS:HE3	1.89	0.72
1:A:39:THR:HG23	1:A:63:ILE:HD13	1.71	0.71
1:B:64:MSE:HE3	2:B:391:HOH:O	1.91	0.70
1:A:131:PRO:HB2	1:A:134:GLU:HG3	1.73	0.70
1:B:233:VAL:HG21	1:B:334:LEU:CD2	2.22	0.70
1:A:70:LEU:HD23	1:A:133:PRO:HG3	1.72	0.70
1:A:175:THR:O	1:A:178:ASP:HB2	1.93	0.69
1:A:17:ILE:HG13	1:A:18:LYS:H	1.56	0.69
1:B:157:ASP:HA	1:B:160:LEU:HD12	1.75	0.69
1:A:172:THR:HG22	1:A:173:GLY:O	1.93	0.68
1:A:297:PRO:HB3	1:A:343:MSE:CE	2.24	0.67
1:B:1:MSE:HE2	1:B:369:TYR:CE2	2.30	0.67
1:A:131:PRO:HB2	1:A:134:GLU:CG	2.25	0.66
1:A:20:ALA:O	1:A:24:LEU:HD23	1.96	0.66
1:B:135:GLU:O	1:B:138:ARG:HG2	1.95	0.66
1:A:297:PRO:HG3	1:A:343:MSE:HB2	1.77	0.65
1:B:1:MSE:HE2	1:B:369:TYR:HE2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:HIS:CE1	1:B:192:VAL:HG23	2.32	0.65
1:A:327:TYR:O	1:A:331:LYS:HB2	1.96	0.65
1:A:361:GLU:HB3	1:A:374:PRO:HG3	1.78	0.65
1:A:82:ASP:OD1	1:A:112:HIS:NE2	2.29	0.64
1:B:200:LYS:HD3	1:B:278:HIS:CD2	2.33	0.64
1:B:335:THR:O	1:B:337:PRO:HD3	1.97	0.64
1:A:71:ALA:HB1	1:B:78:LEU:HD22	1.80	0.63
1:A:12:THR:OG1	1:A:15:GLU:HG3	1.99	0.63
1:B:234:GLN:HG2	1:B:258:ARG:HB3	1.81	0.62
1:B:95:VAL:HB	1:B:102:THR:HG23	1.82	0.62
1:B:281:LEU:HD11	1:B:299:LEU:HD12	1.81	0.62
1:B:174:ASN:ND2	1:B:176:ALA:HB3	2.16	0.61
1:A:204:LEU:O	1:A:205:THR:C	2.44	0.61
1:B:358:ARG:HD3	1:B:375:ASP:O	2.01	0.60
1:B:66:GLU:HB2	2:B:391:HOH:O	2.00	0.60
1:A:86:LYS:O	1:A:89:LYS:NZ	2.34	0.60
1:B:177:ILE:HD11	1:B:289:GLU:O	2.02	0.60
1:B:90:PRO:HD2	1:B:114:ILE:HD13	1.83	0.60
1:A:95:VAL:CG1	1:A:102:THR:HG23	2.31	0.59
1:B:347:SER:O	1:B:349:PRO:HD3	2.02	0.59
1:A:39:THR:HG23	1:A:63:ILE:HD12	1.84	0.59
1:B:204:LEU:CD1	1:B:219:MSE:SE	3.00	0.59
1:B:225:ARG:HG2	1:B:225:ARG:HH11	1.67	0.58
1:B:66:GLU:O	1:B:68:GLN:HG2	2.04	0.58
1:B:231:GLU:HA	1:B:258:ARG:NH2	2.19	0.58
1:B:331:LYS:HA	1:B:334:LEU:HD12	1.86	0.57
1:A:59:PHE:CZ	1:A:88:ILE:HG13	2.40	0.57
1:B:216:MSE:SE	1:B:245:VAL:HG22	2.55	0.57
1:B:84:LEU:CD1	1:B:88:ILE:HD12	2.36	0.56
1:B:192:VAL:O	1:B:196:VAL:HG23	2.05	0.56
1:A:361:GLU:CB	1:A:374:PRO:HG3	2.35	0.56
1:B:227:VAL:O	1:B:258:ARG:NH2	2.38	0.56
1:B:193:LEU:HD13	1:B:276:LYS:HD3	1.86	0.56
1:B:84:LEU:HD12	1:B:88:ILE:HD12	1.88	0.56
1:A:20:ALA:HB3	1:A:21:PRO:HD3	1.89	0.55
1:B:241:LEU:HD22	1:B:241:LEU:H	1.71	0.55
1:A:297:PRO:HB3	1:A:343:MSE:HE3	1.88	0.54
1:A:267:VAL:HG12	1:A:271:HIS:NE2	2.23	0.54
1:A:305:THR:O	1:A:306:GLU:C	2.51	0.54
1:A:196:VAL:HG11	1:A:201:MSE:HB2	1.90	0.54
1:A:268:ILE:O	1:A:272:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:O	1:A:196:VAL:HG23	2.08	0.53
1:A:39:THR:HG22	1:A:39:THR:O	2.08	0.53
1:A:71:ALA:CB	1:B:78:LEU:HD22	2.39	0.53
1:A:13:ARG:HD3	1:A:45:MSE:O	2.09	0.52
1:B:361:GLU:OE1	1:B:374:PRO:HB3	2.09	0.52
1:A:183:THR:HG21	1:A:271:HIS:CD2	2.45	0.52
1:A:81:LEU:HD13	1:A:105:GLY:CA	2.40	0.52
1:A:267:VAL:HG12	1:A:271:HIS:CD2	2.44	0.52
1:B:10:PHE:O	1:B:38:VAL:HA	2.09	0.52
1:A:18:LYS:HD3	1:A:96:HIS:CE1	2.45	0.52
1:A:177:ILE:HG12	1:A:351:GLY:HA3	1.91	0.52
1:A:93:VAL:HG23	1:A:114:ILE:HG21	1.92	0.51
1:A:202:ILE:HG23	1:A:235:VAL:HG22	1.92	0.51
1:B:13:ARG:N	1:B:14:PRO:CD	2.74	0.51
1:A:297:PRO:HB3	1:A:343:MSE:HE2	1.91	0.51
1:B:159:LEU:HD22	1:B:164:LYS:HD2	1.92	0.51
1:A:123:LEU:HB2	1:A:138:ARG:HH11	1.75	0.51
1:A:172:THR:CG2	1:A:355:ALA:HB1	2.41	0.51
1:A:135:GLU:HA	1:A:138:ARG:HH21	1.75	0.51
1:B:80:ARG:HB3	1:B:80:ARG:NH1	2.25	0.51
1:B:355:ALA:O	1:B:359:ILE:HG13	2.10	0.50
1:B:80:ARG:HB3	1:B:80:ARG:HH11	1.76	0.50
1:A:8:THR:CG2	1:A:19:MSE:HE3	2.42	0.50
1:B:225:ARG:NH2	1:B:324:GLU:OE1	2.45	0.50
1:B:333:LEU:CD2	1:B:343:MSE:HE3	2.29	0.50
1:B:362:GLU:OE2	1:B:374:PRO:HD2	2.11	0.49
1:A:17:ILE:HD13	1:A:267:VAL:HG11	1.95	0.49
1:B:317:LYS:HD3	1:B:329:LEU:HD22	1.95	0.49
1:A:136:LEU:HD11	1:B:143:ALA:O	2.13	0.49
1:B:176:ALA:HB1	1:B:290:GLU:OE2	2.13	0.49
1:B:219:MSE:HE2	1:B:301:LEU:HD13	1.95	0.49
1:A:70:LEU:CD2	1:A:133:PRO:HG3	2.41	0.48
1:B:234:GLN:HG2	1:B:258:ARG:CB	2.42	0.48
1:A:282:THR:O	1:A:301:LEU:HG	2.13	0.48
1:A:22:LEU:HA	1:A:356:SER:HB3	1.94	0.48
1:A:156:LYS:HE3	1:A:160:LEU:HD11	1.94	0.48
1:A:120:GLU:HA	1:A:151:PRO:HG3	1.95	0.48
1:B:224:ARG:O	1:B:225:ARG:C	2.56	0.48
1:B:136:LEU:HG	1:B:140:MSE:HE2	1.95	0.48
1:B:341:LYS:CE	1:B:345:GLN:HE22	2.21	0.48
1:B:98:ASP:HB3	1:B:138:ARG:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:O	1:A:49:VAL:HG23	2.13	0.47
1:B:29:TYR:CD2	1:B:364:LEU:HD11	2.49	0.47
1:B:62:ASN:OD1	1:B:80:ARG:NH2	2.47	0.47
1:B:204:LEU:HD12	1:B:205:THR:H	1.79	0.47
1:A:156:LYS:HD2	1:A:169:ILE:HB	1.96	0.47
1:B:258:ARG:HG3	1:B:258:ARG:HH11	1.79	0.47
1:A:20:ALA:N	1:A:21:PRO:CD	2.78	0.47
1:A:20:ALA:N	1:A:21:PRO:HD2	2.30	0.47
1:B:281:LEU:CD1	1:B:299:LEU:HD12	2.44	0.47
1:A:183:THR:HG21	1:A:271:HIS:CG	2.50	0.46
1:A:39:THR:HG21	1:A:101:THR:CG2	2.45	0.46
1:A:332:GLN:O	1:A:336:ASP:HB2	2.14	0.46
1:B:223:ILE:O	1:B:227:VAL:HG23	2.15	0.46
1:A:202:ILE:HD11	1:A:281:LEU:HD13	1.97	0.46
1:B:20:ALA:N	1:B:21:PRO:CD	2.79	0.46
1:B:225:ARG:HG2	1:B:225:ARG:NH1	2.26	0.46
1:A:85:PHE:CE1	1:A:109:ALA:HB2	2.51	0.46
1:A:236:VAL:HG11	1:A:273:PHE:CD2	2.50	0.46
1:A:238:PRO:HB3	1:A:264:PRO:HA	1.98	0.46
1:B:285:GLY:HA3	1:B:307:ARG:HH21	1.79	0.46
1:B:317:LYS:HZ2	1:B:317:LYS:HG3	1.63	0.46
1:B:331:LYS:HA	1:B:334:LEU:CD1	2.46	0.46
1:A:199:ASP:O	1:A:200:LYS:C	2.59	0.46
1:B:14:PRO:O	1:B:18:LYS:HE3	2.14	0.46
1:B:150:ALA:HB1	1:B:155:ALA:HB3	1.98	0.46
1:A:125:THR:HG21	1:A:130:SER:O	2.14	0.45
1:A:135:GLU:OE1	1:A:138:ARG:NH2	2.49	0.45
1:B:313:ALA:HB2	1:B:349:PRO:HG3	1.98	0.45
1:A:17:ILE:O	1:A:19:MSE:N	2.49	0.45
1:B:25:GLU:HA	1:B:28:LYS:HE3	1.98	0.45
1:B:43:ARG:HG2	1:B:60:ASP:OD2	2.17	0.45
1:B:190:HIS:ND1	1:B:192:VAL:HG23	2.32	0.45
1:B:204:LEU:HD12	1:B:205:THR:N	2.31	0.45
1:B:199:ASP:O	1:B:200:LYS:C	2.58	0.45
1:B:317:LYS:HD3	1:B:329:LEU:HD13	1.99	0.45
1:A:266:GLU:O	1:A:267:VAL:C	2.59	0.45
1:A:275:ALA:O	1:A:296:LYS:HE3	2.17	0.45
1:B:125:THR:CG2	1:B:127:ASN:H	2.27	0.45
1:B:335:THR:OG1	1:B:336:ASP:N	2.50	0.45
1:A:131:PRO:CG	1:A:134:GLU:HB2	2.44	0.44
1:B:329:LEU:O	1:B:332:GLN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLN:CD	1:B:339:GLU:HG3	2.42	0.44
1:A:302:ARG:O	1:A:318:LEU:HD22	2.17	0.44
1:B:223:ILE:HG23	1:B:235:VAL:HG21	1.99	0.44
1:A:62:ASN:O	1:A:80:ARG:NH2	2.51	0.44
1:B:174:ASN:HD21	1:B:176:ALA:HB3	1.83	0.44
1:A:266:GLU:O	1:A:269:ASP:N	2.51	0.44
1:B:307:ARG:HB3	1:B:350:TYR:OH	2.18	0.43
1:A:272:ASN:O	1:A:275:ALA:HB3	2.19	0.43
1:A:70:LEU:N	1:A:70:LEU:HD12	2.33	0.43
1:A:301:LEU:HD23	1:A:319:ALA:HB3	2.01	0.43
1:B:158:ASN:O	1:B:162:GLU:HG3	2.18	0.43
1:B:1:MSE:HE1	1:B:31:GLU:HA	2.00	0.43
1:B:278:HIS:CE1	1:B:340:TYR:CE1	3.06	0.43
1:B:233:VAL:HG21	1:B:334:LEU:HD21	1.99	0.43
1:B:237:TYR:CE1	1:B:239:VAL:HG13	2.53	0.43
1:B:1:MSE:CE	1:B:31:GLU:HA	2.48	0.43
1:A:43:ARG:HH21	1:A:57:PRO:CG	2.14	0.43
1:A:129:TYR:CE2	1:B:113:GLN:HG3	2.53	0.43
1:B:128:LYS:HE2	1:B:128:LYS:HB2	1.78	0.43
1:B:225:ARG:HH11	1:B:225:ARG:CG	2.32	0.43
1:A:163:ASN:HB2	1:B:161:LYS:O	2.19	0.42
1:A:88:ILE:N	1:A:88:ILE:HD13	2.34	0.42
1:B:135:GLU:OE1	1:B:138:ARG:HD2	2.20	0.42
1:B:135:GLU:OE1	1:B:138:ARG:NH1	2.52	0.42
1:B:151:PRO:HD2	1:B:155:ALA:CB	2.49	0.42
1:A:267:VAL:HG12	1:A:271:HIS:HE2	1.83	0.42
1:A:223:ILE:O	1:A:224:ARG:C	2.62	0.42
1:A:325:ASN:O	1:A:329:LEU:HD23	2.18	0.42
1:A:188:TYR:HB3	1:A:276:LYS:NZ	2.34	0.42
1:A:125:THR:O	1:A:125:THR:HG22	2.19	0.42
1:A:324:GLU:O	1:A:328:GLN:HG2	2.19	0.42
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.79	0.42
1:A:26:LEU:HD22	1:A:32:ILE:HG21	2.01	0.42
1:B:89:LYS:HA	1:B:89:LYS:HD2	1.89	0.42
1:B:64:MSE:HE2	1:B:68:GLN:CD	2.45	0.42
1:A:147:LEU:HD22	1:A:170:PHE:HE1	1.85	0.42
1:A:14:PRO:O	1:A:17:ILE:HG13	2.20	0.41
1:B:192:VAL:HG21	1:B:262:ILE:HG21	2.01	0.41
1:A:201:MSE:HE2	1:A:236:VAL:HG21	2.02	0.41
1:A:348:ASN:HA	1:A:349:PRO:HD3	1.84	0.41
1:B:165:LYS:HB3	1:B:167:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CE1	1:A:248:ALA:HA	2.55	0.41
1:B:20:ALA:HB3	1:B:21:PRO:HD3	2.02	0.41
1:B:204:LEU:HD21	1:B:219:MSE:SE	2.71	0.41
1:A:13:ARG:N	1:A:14:PRO:CD	2.84	0.41
1:A:161:LYS:O	1:B:163:ASN:HB2	2.21	0.41
1:A:263:GLU:OE2	1:A:264:PRO:HD2	2.20	0.41
1:B:338:ASP:O	1:B:339:GLU:C	2.64	0.41
1:B:70:LEU:H	1:B:70:LEU:HD22	1.86	0.40
1:B:150:ALA:HA	1:B:151:PRO:HD3	1.94	0.40
1:B:378:THR:HG22	1:B:379:GLY:N	2.35	0.40
1:A:81:LEU:HD13	1:A:105:GLY:HA2	2.03	0.40
1:B:352:ASP:O	1:B:354:GLU:HG2	2.21	0.40
1:A:263:GLU:HG3	1:A:264:PRO:HD2	2.04	0.40
1:A:69:THR:N	1:A:72:GLU:OE1	2.49	0.40
1:A:223:ILE:O	1:A:227:VAL:HG23	2.21	0.40
1:A:269:ASP:O	1:A:273:PHE:HD1	2.05	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	344/388 (89%)	311 (90%)	27 (8%)	6 (2%)	7	26
1	B	367/388 (95%)	346 (94%)	20 (5%)	1 (0%)	36	65
All	All	711/776 (92%)	657 (92%)	47 (7%)	7 (1%)	12	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	267	VAL

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Mol	Chain	Res	Type
1	B	254	GLY
1	A	11	GLY
1	A	167	ASP
1	A	17	ILE
1	A	181	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	256/323 (79%)	231 (90%)	25 (10%)	7	25
1	B	300/323 (93%)	272 (91%)	28 (9%)	8	27
All	All	556/646 (86%)	503 (90%)	53 (10%)	8	26

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	25	GLU
1	A	43	ARG
1	A	49	VAL
1	A	73	ILE
1	A	78	LEU
1	A	80	ARG
1	A	88	ILE
1	A	101	THR
1	A	102	THR
1	A	128	LYS
1	A	134	GLU
1	A	183	THR
1	A	202	ILE
1	A	267	VAL
1	A	290	GLU
1	A	293	SER
1	A	306	GLU

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Mol	Chain	Res	Type
1	A	321	THR
1	A	322	ASP
1	A	336	ASP
1	A	343	MSE
1	A	362	GLU
1	A	364	LEU
1	A	373	GLN
1	B	5	LYS
1	B	8	THR
1	B	17	ILE
1	B	22	LEU
1	B	32	ILE
1	B	43	ARG
1	B	44	GLN
1	B	48	GLN
1	B	75	SER
1	B	78	LEU
1	B	80	ARG
1	B	93	VAL
1	B	113	GLN
1	B	125	THR
1	B	162	GLU
1	B	225	ARG
1	B	233	VAL
1	B	239	VAL
1	B	261	LEU
1	B	293	SER
1	B	315	THR
1	B	317	LYS
1	B	318	LEU
1	B	343	MSE
1	B	356	SER
1	B	372	GLU
1	B	376	SER
1	B	378	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	96	HIS
1	A	148	HIS

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Mol	Chain	Res	Type
1	A	190	HIS
1	A	234	GLN
1	A	272	ASN
1	A	288	GLN
1	A	328	GLN
1	A	373	GLN
1	B	139	GLN
1	B	163	ASN
1	B	345	GLN
1	B	366	HIS

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 ⓘ

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	347/388 (89%)	1.01	68 (19%) 3 2	23, 62, 107, 138	0
1	B	361/388 (93%)	0.22	11 (3%) 52 43	16, 36, 66, 103	0
All	All	708/776 (91%)	0.61	79 (11%) 10 9	16, 45, 98, 138	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	TYR	7.7
1	B	167	ASP	5.0
1	A	191	PRO	4.9
1	A	315	THR	4.5
1	A	335	THR	4.4
1	A	232	ASP	4.4
1	A	303	ASP	4.4
1	A	286	GLY	4.3
1	A	310	GLY	4.1
1	B	215	PRO	4.0
1	A	255	ASP	3.8
1	B	255	ASP	3.6
1	A	344	SER	3.5
1	A	62	ASN	3.4
1	A	377	PHE	3.4
1	A	326	ILE	3.3
1	B	354	GLU	3.2
1	A	277	SER	3.1
1	A	319	ALA	3.1
1	A	187	GLY	3.0
1	A	265	LEU	3.0
1	A	304	THR	3.0
1	B	232	ASP	3.0
1	B	126	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	376	SER	2.9
1	A	205	THR	2.9
1	A	338	ASP	2.9
1	A	250	HIS	2.9
1	A	192	VAL	2.8
1	A	238	PRO	2.8
1	A	293	SER	2.8
1	A	44	GLN	2.7
1	A	251	LYS	2.7
1	A	332	GLN	2.7
1	A	311	VAL	2.7
1	A	378	THR	2.6
1	A	247	GLU	2.6
1	A	40	ALA	2.6
1	A	256	SER	2.6
1	A	302	ARG	2.6
1	A	252	HIS	2.6
1	A	193	LEU	2.6
1	A	257	ASP	2.6
1	A	375	ASP	2.6
1	A	317	LYS	2.5
1	B	338	ASP	2.4
1	A	346	ALA	2.4
1	B	305	THR	2.4
1	A	352	ASP	2.4
1	A	42	HIS	2.4
1	A	243	PRO	2.4
1	A	321	THR	2.4
1	A	54	HIS	2.4
1	A	305	THR	2.3
1	A	330	ALA	2.3
1	A	264	PRO	2.3
1	A	351	GLY	2.3
1	A	267	VAL	2.3
1	A	228	GLY	2.3
1	A	266	GLU	2.2
1	A	249	ALA	2.2
1	A	316	LEU	2.2
1	A	341	LYS	2.2
1	A	336	ASP	2.2
1	A	339	GLU	2.2
1	B	229	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	287	VAL	2.2
1	A	323	GLU	2.2
1	A	262	ILE	2.2
1	A	186	ASP	2.2
1	A	188	TYR	2.1
1	A	342	LYS	2.1
1	A	288	GLN	2.1
1	B	250	HIS	2.1
1	A	47	ASP	2.1
1	A	292	PRO	2.0
1	A	294	LEU	2.0
1	A	299	LEU	2.0
1	B	206	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.