



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 2VF4 / pdb_00002vf4
Title : E. coli glucosamine-6-P synthase
Authors : Mouilleron, S.; Golinelli-Pimpaneau, B.
Deposited on : 2007-10-30
Resolution : 2.95 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

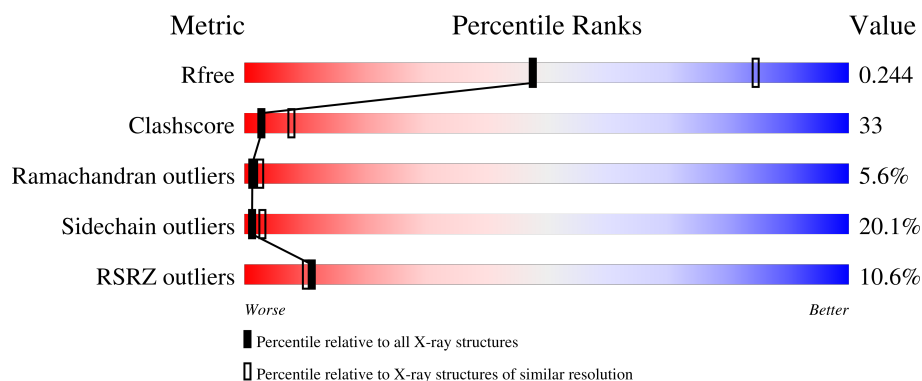
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

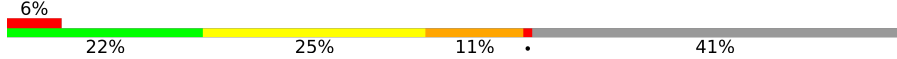
The reported resolution of this entry is 2.95 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	X	608	 6% 22% 25% 11% 41%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2785 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 GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINO-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	359	Total	C	N	O	S	0	2	0
			2774	1755	475	532	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	11	Total	O	0	0
			11	11		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.70Å 144.70Å 171.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.95 15.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.95) 98.8 (15.00-2.95)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.219 , 0.257 0.196 , 0.244	Depositor DCC
R_{free} test set	739 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.019 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.005 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2785	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 i

5.1 Standard geometry i

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	X	1.37	12/2830 (0.4%)	1.48	29/3831 (0.8%)

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	X	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	324	VAL	CA-CB	-9.27	1.42	1.54
1	X	308	MET	SD-CE	6.42	1.95	1.79
1	X	597	GLN	CA-C	5.91	1.60	1.52
1	X	593	THR	CA-CB	-5.83	1.44	1.53
1	X	514	MET	SD-CE	-5.47	1.65	1.79
1	X	316	SER	CA-C	5.32	1.59	1.52
1	X	492	ILE	CA-CB	-5.28	1.48	1.54
1	X	574	ILE	CA-CB	-5.27	1.47	1.54
1	X	470	LEU	CA-C	-5.17	1.46	1.52
1	X	299	ALA	CA-CB	-5.16	1.45	1.53
1	X	557	ASP	CG-OD1	5.12	1.35	1.25
1	X	494	ALA	CA-C	5.06	1.59	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	309	VAL	N-CA-C	-9.61	102.00	110.74
1	X	518	VAL	CB-CA-C	-9.35	95.89	110.95
1	X	488	GLU	N-CA-C	8.34	120.14	111.14
1	X	556	SER	N-CA-C	-7.10	99.94	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	558	ASN	N-CA-C	7.08	121.63	112.92
1	X	248	TYR	N-CA-C	7.00	119.77	110.53
1	X	270	ARG	N-CA-C	-6.67	105.70	114.31
1	X	549	GLN	N-CA-C	-6.49	104.25	111.71
1	X	299	ALA	N-CA-C	6.47	117.12	108.38
1	X	600	ASN	N-CA-C	6.30	119.86	111.30
1	X	595	VAL	N-CA-C	6.27	117.77	110.62
1	X	394	GLY	N-CA-C	-6.21	98.45	113.18
1	X	476	TYR	CA-C-N	-6.12	113.83	119.82
1	X	476	TYR	C-N-CA	-6.12	113.83	119.82
1	X	595	VAL	CB-CA-C	-5.96	104.23	112.04
1	X	375	ASN	N-CA-C	5.82	119.51	111.71
1	X	329	GLU	CA-C-N	5.75	128.24	120.65
1	X	329	GLU	C-N-CA	5.75	128.24	120.65
1	X	320	ILE	CB-CA-C	-5.52	104.43	110.78
1	X	256	ILE	N-CA-C	-5.45	105.40	110.53
1	X	505	GLY	CA-C-N	5.31	125.38	119.32
1	X	505	GLY	C-N-CA	5.31	125.38	119.32
1	X	428	SER	N-CA-C	-5.31	105.16	111.69
1	X	571	ILE	N-CA-C	5.29	118.07	112.83
1	X	486	LEU	N-CA-C	-5.28	105.44	111.14
1	X	538	ALA	N-CA-C	5.25	117.75	111.71
1	X	524	GLU	N-CA-C	-5.10	105.18	111.40
1	X	557	ASP	CA-C-N	-5.08	114.51	122.65
1	X	557	ASP	C-N-CA	-5.08	114.51	122.65

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	272	SER	Peptide
1	X	287	GLU	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	X	2774	0	2799	184	0
2	X	11	0	0	0	0
All	All	2785	0	2799	184	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 33.

All (184) 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:X:472:ARG:HG2	1:X:473:GLY:N	1.70	1.02
1:X:472:ARG:HG2	1:X:473:GLY:H	1.25	0.96
1:X:341:SER:HB3	1:X:367:TYR:CD2	2.02	0.93
1:X:412:LEU:O	1:X:416:VAL:HG23	1.72	0.89
1:X:348:GLN:HE21	1:X:349:SER:N	1.70	0.89
1:X:443:ARG:HD3	1:X:567:VAL:HG12	1.52	0.88
1:X:466:HIS:CB	1:X:514:MET:HG2	2.04	0.88
1:X:474:ASP:OD2	1:X:573:PRO:HG2	1.72	0.88
1:X:466:HIS:HB2	1:X:514:MET:HG2	1.55	0.87
1:X:474:ASP:OD2	1:X:573:PRO:CG	2.22	0.87
1:X:346:LEU:HD11	1:X:412:LEU:HD11	1.59	0.84
1:X:348:GLN:HE21	1:X:348:GLN:C	1.86	0.84
1:X:362:SER:HB2	1:X:367:TYR:CD1	2.14	0.82
1:X:297:ILE:O	1:X:298:LEU:HD23	1.78	0.82
1:X:430:GLU:O	1:X:434:VAL:HG23	1.79	0.82
1:X:341:SER:HB3	1:X:367:TYR:HD2	1.42	0.81
1:X:328:SER:HB3	1:X:354:ASP:OD2	1.81	0.80
1:X:472:ARG:CG	1:X:473:GLY:H	1.95	0.79
1:X:466:HIS:HB2	1:X:514:MET:CG	2.11	0.79
1:X:305:ASN:O	1:X:309:VAL:HG23	1.81	0.78
1:X:263:ILE:HG21	1:X:440:LEU:HD23	1.65	0.76
1:X:374:CYS:SG	1:X:375:ASN:N	2.59	0.75
1:X:261:ASN:O	1:X:264:LYS:N	2.20	0.75
1:X:362:SER:HB2	1:X:367:TYR:HD1	1.50	0.74
1:X:262:ALA:HA	1:X:265:ASN:HD22	1.52	0.74
1:X:404:ALA:O	1:X:408:GLN:HG3	1.87	0.73
1:X:577:THR:O	1:X:581:GLN:HG3	1.89	0.73
1:X:548:ASP:OD1	1:X:550:ASP:HB2	1.90	0.72
1:X:457:LEU:HD11	1:X:461:PHE:HE1	1.54	0.71
1:X:450:GLN:CG	1:X:453:ARG:HH21	2.03	0.70
1:X:466:HIS:CB	1:X:514:MET:CG	2.69	0.70
1:X:450:GLN:HG2	1:X:453:ARG:HH21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:549:GLN:HE21	1:X:565:PRO:HA	1.56	0.69
1:X:572:ALA:HB3	1:X:573:PRO:HD3	1.75	0.68
1:X:294:HIS:CD2	1:X:338:ARG:HG2	2.28	0.67
1:X:443:ARG:O	1:X:446:GLN:HB2	1.95	0.66
1:X:411:VAL:O	1:X:412:LEU:C	2.37	0.65
1:X:484:LEU:HG	1:X:488:GLU:OE1	1.97	0.65
1:X:600:ASN:C	1:X:601:LEU:HG	2.22	0.65
1:X:466:HIS:HB3	1:X:514:MET:HG2	1.77	0.65
1:X:341:SER:HB3	1:X:367:TYR:CE2	2.31	0.65
1:X:348:GLN:NE2	1:X:349:SER:N	2.46	0.62
1:X:261:ASN:O	1:X:264:LYS:HB2	1.99	0.62
1:X:344:ILE:HA	1:X:371:LEU:O	2.00	0.62
1:X:256:ILE:HG12	1:X:402:THR:HG21	1.82	0.62
1:X:443:ARG:HA	1:X:446:GLN:HG3	1.82	0.62
1:X:450:GLN:HG2	1:X:453:ARG:NH2	2.15	0.61
1:X:376:VAL:O	1:X:382:VAL:HG21	2.00	0.61
1:X:371:LEU:HD21	1:X:389:LEU:HD12	1.83	0.61
1:X:278:LEU:HD12	1:X:418:LYS:HB2	1.84	0.60
1:X:578:VAL:N	1:X:579:PRO:CD	2.65	0.59
1:X:443:ARG:NH1	1:X:446:GLN:HE21	2.00	0.59
1:X:278:LEU:HB2	1:X:418:LYS:HD3	1.84	0.58
1:X:440:LEU:HB3	1:X:441:PRO:HD3	1.86	0.58
1:X:271:ILE:HG21	1:X:438:GLN:HE21	1.68	0.58
1:X:471:GLY:HA3	1:X:476:TYR:HA	1.84	0.58
1:X:310:SER:CB	1:X:412:LEU:HD22	2.34	0.58
1:X:347:SER:O	1:X:374:CYS:HA	2.04	0.57
1:X:512:ALA:HA	1:X:540:GLY:O	2.05	0.57
1:X:414:MET:O	1:X:417:ALA:N	2.37	0.57
1:X:433:ILE:O	1:X:437:LEU:HB2	2.06	0.56
1:X:443:ARG:NH1	1:X:443:ARG:HG2	2.20	0.56
1:X:264:LYS:O	1:X:267:LEU:HB2	2.05	0.56
1:X:328:SER:CB	1:X:354:ASP:OD2	2.54	0.56
1:X:475:GLN:HG3	1:X:520:ALA:HB3	1.86	0.56
1:X:486:LEU:HD12	1:X:490:SER:OG	2.05	0.56
1:X:425:LEU:O	1:X:427:ALA:N	2.34	0.56
1:X:342:LEU:HD12	1:X:369:GLY:O	2.06	0.55
1:X:446:GLN:O	1:X:449:SER:OG	2.22	0.55
1:X:409:LEU:HD13	1:X:574:ILE:HG12	1.88	0.55
1:X:506:PRO:O	1:X:507:LEU:C	2.46	0.55
1:X:578:VAL:N	1:X:579:PRO:HD2	2.21	0.55
1:X:563:GLU:O	1:X:564:MET:HE3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:259:GLN:N	1:X:260:PRO:HD2	2.22	0.55
1:X:421:ARG:C	1:X:423:LYS:H	2.14	0.55
1:X:313:TRP:CE3	1:X:413:LEU:HD13	2.42	0.55
1:X:262:ALA:HA	1:X:265:ASN:ND2	2.21	0.54
1:X:450:GLN:O	1:X:451:ASP:C	2.49	0.54
1:X:297:ILE:HD11	1:X:322:CYS:SG	2.48	0.54
1:X:310:SER:HB2	1:X:412:LEU:HD22	1.89	0.54
1:X:426:ASP:C	1:X:428:SER:H	2.15	0.54
1:X:474:ASP:OD2	1:X:573:PRO:HG3	2.07	0.53
1:X:278:LEU:O	1:X:281:LEU:HB2	2.08	0.53
1:X:477:PRO:HA	1:X:480:LEU:HD12	1.90	0.53
1:X:443:ARG:HG2	1:X:443:ARG:HH11	1.74	0.53
1:X:564:MET:HA	1:X:564:MET:HE2	1.90	0.53
1:X:259:GLN:O	1:X:263:ILE:HG13	2.09	0.53
1:X:393:ALA:O	1:X:403:LYS:HE3	2.09	0.52
1:X:250:HIS:HD2	1:X:585:TYR:OH	1.92	0.52
1:X:351:GLU:OE2	1:X:380:SER:N	2.43	0.52
1:X:302:THR:CG2	1:X:405:PHE:CD1	2.92	0.52
1:X:256:ILE:HA	1:X:259:GLN:NE2	2.25	0.52
1:X:261:ASN:O	1:X:262:ALA:C	2.54	0.51
1:X:297:ILE:HA	1:X:344:ILE:O	2.10	0.51
1:X:378:GLY:O	1:X:383:ARG:NH1	2.41	0.51
1:X:299:ALA:HA	1:X:355:THR:CG2	2.41	0.51
1:X:298:LEU:HD11	1:X:330:PHE:CD2	2.46	0.51
1:X:263:ILE:HG21	1:X:440:LEU:CD2	2.38	0.50
1:X:372:ALA:HB2	1:X:385:SER:OG	2.11	0.50
1:X:481:GLU:OE2	1:X:485:LYS:NZ	2.35	0.50
1:X:407:THR:O	1:X:410:THR:HB	2.10	0.50
1:X:548:ASP:CG	1:X:550:ASP:HB2	2.37	0.50
1:X:462:SER:HA	1:X:587:VAL:HG13	1.93	0.50
1:X:310:SER:HB3	1:X:412:LEU:HD13	1.94	0.49
1:X:598:PRO:HB2	1:X:601:LEU:HD12	1.94	0.49
1:X:532:ASN:O	1:X:535:GLU:HB2	2.12	0.49
1:X:413:LEU:HD23	1:X:437:LEU:CD2	2.42	0.49
1:X:472:ARG:O	1:X:473:GLY:C	2.55	0.49
1:X:476:TYR:CE2	1:X:480:LEU:HD11	2.48	0.49
1:X:457:LEU:HD11	1:X:461:PHE:CE1	2.43	0.48
1:X:525:LEU:O	1:X:526:LEU:C	2.56	0.48
1:X:572:ALA:HB3	1:X:573:PRO:CD	2.44	0.48
1:X:393:ALA:C	1:X:394:GLY:O	2.52	0.48
1:X:311:ARG:HG3	1:X:322:CYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:267:LEU:HD21	1:X:437:LEU:CD1	2.45	0.47
1:X:302:THR:HG22	1:X:405:PHE:HD1	1.79	0.47
1:X:431:HIS:HA	1:X:434:VAL:HG23	1.97	0.47
1:X:472:ARG:CG	1:X:473:GLY:N	2.47	0.47
1:X:371:LEU:HD12	1:X:387:LEU:O	2.15	0.47
1:X:271:ILE:HA	1:X:275:GLN:O	2.14	0.47
1:X:262:ALA:CA	1:X:265:ASN:HD22	2.24	0.46
1:X:447:MET:HE2	1:X:575:PHE:CZ	2.50	0.46
1:X:278:LEU:HD12	1:X:418:LYS:HD3	1.98	0.46
1:X:375:ASN:HD21	1:X:393:ALA:H	1.63	0.46
1:X:274:GLY:O	1:X:275:GLN:HG3	2.16	0.46
1:X:476:TYR:CD2	1:X:476:TYR:C	2.94	0.46
1:X:591:LYS:HB2	1:X:593:THR:HG23	1.97	0.46
1:X:415:LEU:HG	1:X:419:LEU:HD23	1.98	0.46
1:X:475:GLN:O	1:X:478:ILE:N	2.41	0.45
1:X:518:VAL:HG23	1:X:545:VAL:HA	1.97	0.45
1:X:314:PHE:O	1:X:315:GLU:C	2.59	0.45
1:X:466:HIS:HB2	1:X:514:MET:HG3	1.95	0.45
1:X:375:ASN:O	1:X:375:ASN:ND2	2.50	0.45
1:X:425:LEU:H	1:X:425:LEU:HD12	1.81	0.45
1:X:475:GLN:O	1:X:478:ILE:HB	2.17	0.45
1:X:302:THR:CG2	1:X:405:PHE:HD1	2.30	0.45
1:X:557:ASP:OD1	1:X:558:ASN:N	2.48	0.45
1:X:380:SER:HA	1:X:383:ARG:NH2	2.32	0.44
1:X:461:PHE:CE2	1:X:517:ILE:HD11	2.52	0.44
1:X:582:LEU:HD23	1:X:582:LEU:HA	1.79	0.44
1:X:457:LEU:CD1	1:X:461:PHE:HE1	2.26	0.44
1:X:580:LEU:N	1:X:580:LEU:HD23	2.32	0.44
1:X:505:GLY:HA3	1:X:506:PRO:HD3	1.81	0.44
1:X:244:ASP:O	1:X:254:LYS:HE2	2.17	0.44
1:X:357:ALA:HA	1:X:360:ARG:HD2	1.99	0.44
1:X:452:LYS:HD2	1:X:452:LYS:HA	1.64	0.44
1:X:475:GLN:OE1	1:X:475:GLN:HA	2.16	0.44
1:X:265:ASN:C	1:X:267:LEU:H	2.26	0.43
1:X:576:TYR:C	1:X:579:PRO:HD2	2.43	0.43
1:X:256:ILE:HA	1:X:259:GLN:HE21	1.83	0.43
1:X:389:LEU:HD23	1:X:389:LEU:HA	1.86	0.43
1:X:447:MET:HE2	1:X:575:PHE:CE1	2.54	0.43
1:X:343:MET:HG3	1:X:345:THR:HG22	1.99	0.43
1:X:245:LYS:HD3	1:X:249:ARG:O	2.19	0.42
1:X:466:HIS:CB	1:X:514:MET:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:GLU:O	1:X:352:THR:C	2.62	0.42
1:X:270:ARG:HG3	1:X:270:ARG:NH1	2.35	0.42
1:X:440:LEU:HD12	1:X:571:ILE:HD12	2.00	0.42
1:X:276:VAL:HG21	1:X:417:ALA:HB3	2.01	0.41
1:X:299:ALA:HB2	1:X:346:LEU:O	2.20	0.41
1:X:511:ASP:C	1:X:511:ASP:OD1	2.63	0.41
1:X:583:LEU:HD12	1:X:583:LEU:HA	1.72	0.41
1:X:370:SER:HG	1:X:386:ASP:H	1.64	0.41
1:X:443:ARG:HH12	1:X:446:GLN:HE21	1.66	0.41
1:X:256:ILE:O	1:X:259:GLN:HB2	2.20	0.41
1:X:291:LYS:HE2	1:X:291:LYS:HB3	1.72	0.41
1:X:299:ALA:HA	1:X:355:THR:HG22	2.02	0.41
1:X:326:ILE:O	1:X:327:ALA:C	2.64	0.41
1:X:447:MET:HG2	1:X:578:VAL:HB	2.03	0.41
1:X:259:GLN:HG2	1:X:406:THR:OG1	2.20	0.41
1:X:340:ASN:HB3	1:X:368:LEU:HD11	2.02	0.41
1:X:570:VAL:HG12	1:X:571:ILE:HG23	2.03	0.41
1:X:281:LEU:HB3	1:X:285:ALA:HB2	2.03	0.41
1:X:295:ILE:CG2	1:X:344:ILE:HD11	2.50	0.41
1:X:313:TRP:HH2	1:X:574:ILE:HD11	1.86	0.41
1:X:557:ASP:O	1:X:560:HIS:CE1	2.74	0.41
1:X:345:THR:O	1:X:345:THR:OG1	2.38	0.41
1:X:281:LEU:HD22	1:X:387:LEU:HD22	2.02	0.40
1:X:485:LYS:HD3	1:X:485:LYS:HA	1.95	0.40
1:X:287:GLU:HB3	1:X:288:LEU:H	1.37	0.40
1:X:300:CYS:O	1:X:301:GLY:C	2.65	0.40
1:X:313:TRP:O	1:X:314:PHE:C	2.64	0.40
1:X:411:VAL:C	1:X:413:LEU:N	2.78	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	X	359/608 (59%)	282 (79%)	57 (16%)	20 (6%)	1 2

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	287	GLU
1	X	288	LEU
1	X	348	GLN
1	X	426	ASP
1	X	427	ALA
1	X	340	ASN
1	X	392	ASN
1	X	422	LEU
1	X	425	LEU
1	X	451	ASP
1	X	473	GLY
1	X	261	ASN
1	X	314	PHE
1	X	352	THR
1	X	380	SER
1	X	576	TYR
1	X	301	GLY
1	X	331	ARG
1	X	262	ALA
1	X	404	ALA

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	X	301/500 (60%)	241 (80%)	60 (20%)	1 3

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	256	ILE

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Mol	Chain	Res	Type
1	X	259	GLN
1	X	264	LYS
1	X	270	ARG
1	X	272	SER
1	X	279	SER
1	X	280	GLU
1	X	290	SER
1	X	291	LYS
1	X	293	GLU
1	X	297	ILE
1	X	298	LEU
1	X	302	THR
1	X	308	MET
1	X	324	VAL
1	X	326	ILE
1	X	329	GLU
1	X	333	ARG
1	X	334	LYS
1	X	335	SER
1	X	337	VAL
1	X	341	SER
1	X	344	ILE
1	X	347	SER
1	X	348	GLN
1	X	361	LEU
1	X	364	GLU
1	X	365	LEU
1	X	374	CYS
1	X	381	LEU
1	X	383	ARG
1	X	391	THR
1	X	392	ASN
1	X	399	VAL
1	X	402	THR
1	X	406	THR
1	X	410	THR
1	X	421	ARG
1	X	423	LYS
1	X	426	ASP
1	X	434	VAL
1	X	437	LEU
1	X	440	LEU

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Mol	Chain	Res	Type
1	X	443	ARG
1	X	444	ILE
1	X	450	GLN
1	X	452	LYS
1	X	503	LYS
1	X	513	ASP
1	X	518	VAL
1	X	524	GLU
1	X	537	ARG
1	X	543	LEU
1	X	554	VAL
1	X	556	SER
1	X	564	MET
1	X	570	VAL
1	X	573	PRO
1	X	597	GLN
1	X	601	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	250	HIS
1	X	259	GLN
1	X	265	ASN
1	X	348	GLN
1	X	375	ASN
1	X	438	GLN
1	X	446	GLN
1	X	450	GLN
1	X	504	HIS
1	X	549	GLN
1	X	581	GLN
1	X	597	GLN

5.3.3 RNA ⓘ

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	X	359/608 (59%)	0.52	38 (10%)	11 10	9, 17, 21, 25	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	250	HIS	5.1
1	X	249	ARG	5.0
1	X	388	ALA	4.3
1	X	247	ILE	3.9
1	X	282	GLY	3.9
1	X	272	SER	3.9
1	X	243	GLY	3.8
1	X	399	VAL	3.6
1	X	404	ALA	3.5
1	X	449	SER	3.5
1	X	318	ALA	3.4
1	X	274	GLY	3.1
1	X	255	GLU	3.0
1	X	321	PRO	3.0
1	X	601	LEU	3.0
1	X	400	ALA	3.0
1	X	301	GLY	2.8
1	X	473	GLY	2.8
1	X	253	GLN	2.8
1	X	277	ASP	2.8
1	X	425	LEU	2.7
1	X	392	ASN	2.7
1	X	302	THR	2.7
1	X	284	ASN	2.6
1	X	336	ALA	2.6
1	X	248	TYR	2.5
1	X	382	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	245	LYS	2.4
1	X	257	TYR	2.4
1	X	283	PRO	2.3
1	X	246	GLY	2.3
1	X	275	GLN	2.2
1	X	557	ASP	2.2
1	X	300	CYS	2.2
1	X	387	LEU	2.2
1	X	273	HIS	2.1
1	X	252	MET	2.1
1	X	401[A]	SER	2.1

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.