



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:21 PM GMT

PDB ID : 2VF4  
Title : E. COLI GLUCOSAMINE-6-P SYNTHASE  
Authors : Mouilleron, S.; Golineli-Pimpaneau, B.  
Deposited on : 2007-10-30  
Resolution : 2.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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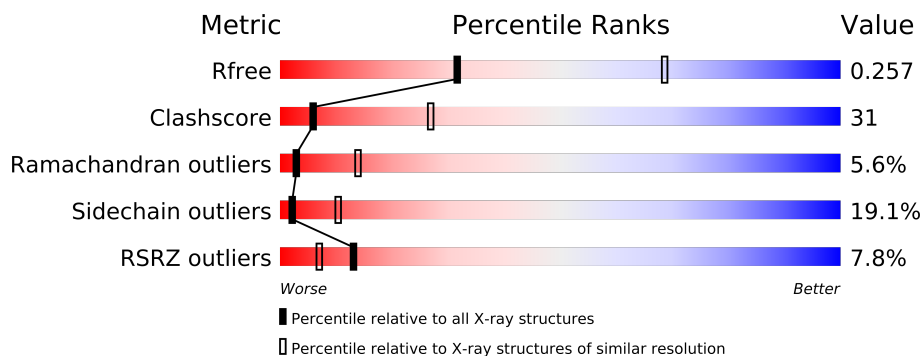
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.95 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))
$R_{free}$	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	X	608	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2785 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLUCOSAMINE--FRUCTOSE-6-PHOSPHATEAMINO-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.

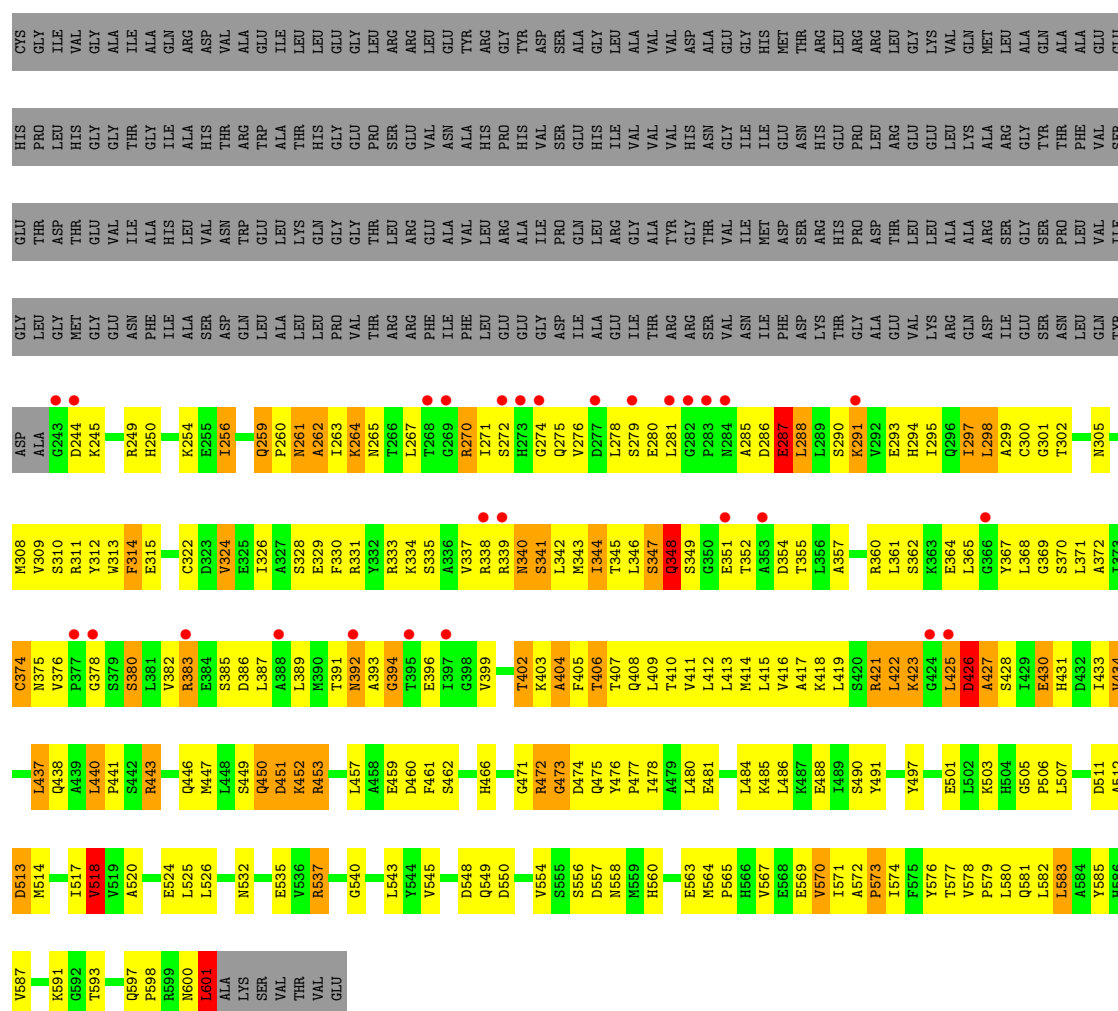
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	11	Total	O	0	0
			11	11		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATEAMINOTRANSFERASE

Chain X: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.70Å 144.70Å 171.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.95 14.97 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.95) 99.7 (14.97-2.95)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.219 , 0.257 0.211 , 0.257	Depositor DCC
$R_{free}$ test set	739 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -10.0	EDS
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
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14602 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	2785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	X	1.10	6/2830 (0.2%)	1.18	15/3831 (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	X	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	569	GLU	CD-OE2	7.16	1.33	1.25
1	X	312	TYR	CE1-CZ	6.71	1.47	1.38
1	X	501	GLU	CD-OE1	6.28	1.32	1.25
1	X	324	VAL	CA-CB	-5.80	1.42	1.54
1	X	300	CYS	CB-SG	-5.71	1.72	1.81
1	X	459	GLU	CD-OE1	5.20	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	518	VAL	CB-CA-C	-8.16	95.89	111.40
1	X	511	ASP	CB-CG-OD2	8.12	125.61	118.30
1	X	453	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	X	601	LEU	CB-CG-CD1	7.09	123.06	111.00
1	X	426	ASP	CB-CG-OD2	6.46	124.11	118.30
1	X	286	ASP	CB-CG-OD2	6.07	123.77	118.30
1	X	513	ASP	CB-CG-OD1	6.03	123.73	118.30
1	X	453	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	X	422	LEU	CA-CB-CG	5.88	128.83	115.30
1	X	394	GLY	N-CA-C	-5.86	98.45	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	537	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	X	308	MET	CG-SD-CE	5.51	109.01	100.20
1	X	472	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	X	583	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	X	460	ASP	CB-CG-OD1	5.12	122.91	118.30

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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	2774	0	2799	174	0
2	X	11	0	0	0	0
All	All	2785	0	2799	174	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (174) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:348:GLN:HE21	1:X:348:GLN:C	1.86	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
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:484:LEU:HG	1:X:488:GLU:OE1	1.97	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:344:ILE:HA	1:X:371:LEU:O	2.00	0.62
1:X:261:ASN:O	1:X:264:LYS:HB2	1.99	0.62
1:X:443:ARG:HA	1:X:446:GLN:HG3	1.82	0.62
1:X:256:ILE:HG12	1:X:402:THR:HG21	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:411:VAL:O	1:X:412:LEU:C	2.37	0.60
1:X:600:ASN:C	1:X:601:LEU:HG	2.22	0.60
1:X:563:GLU:O	1:X:564:MET:HE3	2.01	0.60
1:X:278:LEU:HD12	1:X:418:LYS:HB2	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:443:ARG:HG2	1:X:443:ARG:NH1	2.20	0.56
1:X:433:ILE:O	1:X:437:LEU:HB2	2.06	0.56
1:X:328:SER:CB	1:X:354:ASP:OD2	2.54	0.56
1:X:264:LYS:O	1:X:267:LEU:HB2	2.05	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:446:GLN:O	1:X:449:SER:OG	2.22	0.55
1:X:342:LEU:HD12	1:X:369:GLY:O	2.06	0.55
1:X:409:LEU:HD13	1:X:574:ILE:HG12	1.88	0.55
1:X:578:VAL:N	1:X:579:PRO:HD2	2.21	0.55
1:X:259:GLN:N	1:X:260:PRO:HD2	2.22	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: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: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: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: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:506:PRO:O	1:X:507:LEU:C	2.46	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:421:ARG:C	1:X:423:LYS:H	2.14	0.50
1:X:407:THR:O	1:X:410:THR:HB	2.10	0.50
1:X:462:SER:HA	1:X:587:VAL:HG13	1.93	0.50
1:X:426:ASP:C	1:X:428:SER:H	2.15	0.50
1:X:310:SER:HB3	1:X:412:LEU:HD13	1.94	0.49
1:X:450:GLN:O	1:X:451:ASP:C	2.49	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: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:572:ALA:HB3	1:X:573:PRO:CD	2.44	0.48
1:X:564:MET:HA	1:X:564:MET:HE2	1.96	0.47
1:X:311:ARG:HG3	1:X:322:CYS:HB3	1.97	0.47
1:X:472:ARG:CG	1:X:473:GLY:N	2.47	0.47
1:X:431:HIS:HA	1:X:434:VAL:HG23	1.97	0.47
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:371:LEU:HD12	1:X:387:LEU:O	2.15	0.47
1:X:261:ASN:O	1:X:262:ALA:C	2.54	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: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: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:548:ASP:CG	1:X:550:ASP:HB2	2.37	0.45
1:X:466:HIS:HB2	1:X:514:MET:HG3	1.95	0.45
1:X:375:ASN:ND2	1:X:375:ASN:O	2.50	0.45
1:X:475:GLN:HA	1:X:475:GLN:OE1	2.16	0.45
1:X:475:GLN:O	1:X:478:ILE:HB	2.17	0.45
1:X:425:LEU:H	1:X:425:LEU:HD12	1.81	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:HA	1:X:582:LEU:HD23	1.79	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:457:LEU:CD1	1:X:461:PHE:HE1	2.26	0.44
1:X:580:LEU:HD23	1:X:580:LEU:N	2.32	0.44
1:X:472:ARG:O	1:X:473:GLY:C	2.55	0.44
1:X:505:GLY:HA3	1:X:506:PRO:HD3	1.81	0.44
1:X:343:MET:HE2	1:X:362:SER:HB3	2.00	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:HA	1:X:452:LYS:HD2	1.64	0.44
1:X:525:LEU:O	1:X:526:LEU:C	2.56	0.43
1:X:393:ALA:C	1:X:394:GLY:O	2.52	0.43
1:X:389:LEU:HA	1:X:389:LEU:HD23	1.86	0.43
1:X:256:ILE:HA	1:X:259:GLN:HE21	1.83	0.43
1:X:343:MET:HG3	1:X:345:THR:HG22	1.99	0.43
1:X:466:HIS:CB	1:X:514:MET:HG3	2.49	0.42
1:X:245:LYS:HD3	1:X:249:ARG:O	2.19	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:299:ALA:HB2	1:X:346:LEU:O	2.20	0.41
1:X:276:VAL:HG21	1:X:417:ALA:HB3	2.01	0.41
1:X:583:LEU:HA	1:X:583:LEU:HD12	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:476:TYR:C	1:X:476:TYR:CD2	2.94	0.41
1:X:299:ALA:HA	1:X:355:THR:HG22	2.02	0.41
1:X:447:MET:HG2	1:X:578:VAL:HB	2.03	0.41
1:X:291:LYS:HE2	1:X:291:LYS:HB3	1.72	0.41
1:X:259:GLN:HG2	1:X:406:THR:OG1	2.20	0.41
1:X:570:VAL:HG12	1:X:571:ILE:HG23	2.03	0.41
1:X:340:ASN:HB3	1:X:368:LEU:HD11	2.02	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:281:LEU:HD22	1:X:387:LEU:HD22	2.02	0.40
1:X:485:LYS:HA	1:X:485:LYS:HD3	1.95	0.40
1:X:314:PHE:O	1:X:315:GLU:C	2.59	0.40
1:X:287:GLU:HB3	1:X:288:LEU:H	1.37	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	X	359/608 (59%)	282 (79%)	57 (16%)	20 (6%)	3 14

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%)	244 (81%)	57 (19%)	2 10

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	256	ILE
1	X	259	GLN
1	X	264	LYS
1	X	270	ARG
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	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	339	ARG
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	383	ARG
1	X	391	THR
1	X	392	ASN
1	X	399	VAL
1	X	402	THR
1	X	406	THR
1	X	421	ARG
1	X	423	LYS
1	X	426	ASP
1	X	430	GLU
1	X	434	VAL

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Mol	Chain	Res	Type
1	X	437	LEU
1	X	440	LEU
1	X	443	ARG
1	X	450	GLN
1	X	452	LYS
1	X	491	TYR
1	X	497	TYR
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	570	VAL
1	X	573	PRO
1	X	597	GLN
1	X	601	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	438	GLN
1	X	446	GLN
1	X	450	GLN
1	X	549	GLN
1	X	581	GLN
1	X	597	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	359/608 (59%)	0.49	28 (7%) 13 7	12, 17, 21, 25	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	282	GLY	6.5
1	X	284	ASN	4.8
1	X	283	PRO	4.6
1	X	269	GLY	4.6
1	X	388	ALA	4.3
1	X	272	SER	4.2
1	X	425	LEU	3.9
1	X	378	GLY	3.5
1	X	383	ARG	3.4
1	X	268	THR	3.4
1	X	273	HIS	3.3
1	X	338	ARG	3.2
1	X	279	SER	3.2
1	X	277	ASP	3.2
1	X	377	PRO	3.1
1	X	392	ASN	3.1
1	X	291	LYS	3.1
1	X	274	GLY	3.1
1	X	243	GLY	2.7
1	X	424	GLY	2.7
1	X	366	GLY	2.6
1	X	397	ILE	2.6
1	X	395	THR	2.5
1	X	339	ARG	2.4
1	X	281	LEU	2.3
1	X	244	ASP	2.3
1	X	353	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	351	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.