



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 02:57 pm GMT

PDB ID : 1FP3
Title : CRYSTAL STRUCTURE OF N-ACYL-D-GLUCOSAMINE 2-EPIMERASE
FROM PORCINE KIDNEY
Authors : Itoh, T.; Mikami, B.; Maru, I.; Ohta, Y.; Hashimoto, W.; Murata, K.
Deposited on : 2000-08-30
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

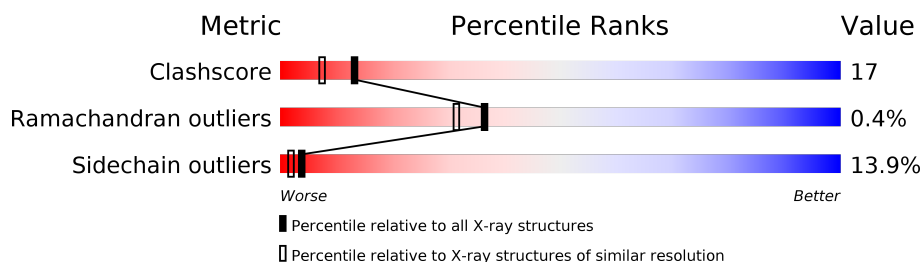
1 Overall quality at a glance

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))
Clashscore	122078	8264 (2.00-2.00)
Ramachandran outliers	120005	8163 (2.00-2.00)
Sidechain outliers	119972	8162 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	402	
1	B	402	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6675 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 N-ACYL-D-GLUCOSAMINE 2-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3265	2075	585	579	26			
1	B	402	Total	C	N	O	S	0	0	0
			3265	2075	585	579	26			

- Molecule 2 is water.

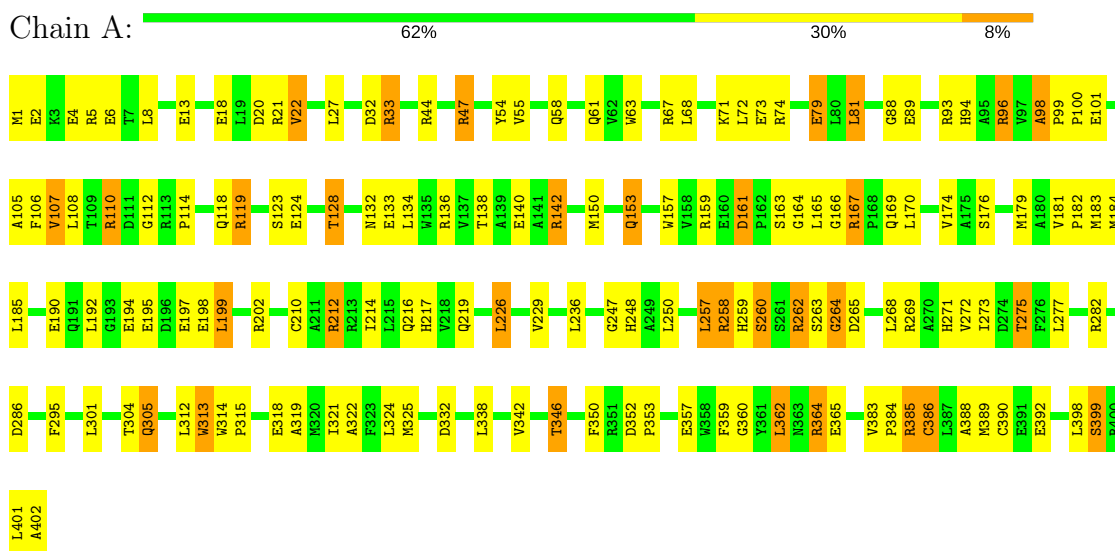
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	67	Total	O	0	0
			67	67		

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 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.

Note EDS was not executed.

• Molecule 1: N-ACYL-D-GLUCOSAMINE 2-EPIMERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 97.19Å 100.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.00	Depositor
% Data completeness (in resolution range)	74.8 (14.97-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.169 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6675	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	A	0.40	0/3354	0.62	0/4527
1	B	0.40	0/3354	0.62	0/4527
All	All	0.40	0/6708	0.62	0/9054

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	ALA	Peptide
1	A	99	PRO	Peptide
1	B	99	PRO	Peptide

5.2 Too-close contacts [i](#)

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	3265	0	3154	119	0
1	B	3265	0	3154	110	0
2	A	78	0	0	7	0
2	B	67	0	0	3	0
All	All	6675	0	6308	223	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 17.

All (223) 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:33:ARG:HH11	1:B:33:ARG:HG2	1.09	1.17
1:B:5:ARG:HH21	1:B:402:ALA:HB2	1.08	1.10
1:A:21:ARG:HH12	1:A:353:PRO:HA	1.24	1.03
1:B:5:ARG:NH2	1:B:402:ALA:HB2	1.84	0.91
1:A:21:ARG:NH1	1:A:353:PRO:HA	1.91	0.85
1:B:33:ARG:NH1	1:B:33:ARG:HG2	1.89	0.85
1:B:279:LEU:HB3	1:B:280:PRO:HD3	1.59	0.85
1:A:385:ARG:O	1:A:389:MET:HG3	1.78	0.83
1:A:258:ARG:N	1:A:325:MET:HE1	1.95	0.81
1:A:295:PHE:CD1	1:A:305:GLN:HG3	2.17	0.80
1:A:192:LEU:HB3	1:A:199:LEU:HD12	1.66	0.78
1:B:33:ARG:HH11	1:B:33:ARG:CG	1.96	0.77
1:A:73:GLU:HG2	1:B:392:GLU:HB3	1.67	0.76
1:B:321:ILE:HD11	1:B:386:CYS:HA	1.67	0.76
1:B:5:ARG:O	1:B:9:GLN:HG3	1.88	0.74
1:A:119:ARG:HH11	1:A:119:ARG:HG2	1.52	0.73
1:B:167:ARG:HB2	1:B:167:ARG:CZ	2.19	0.70
1:B:1:MET:HB3	1:B:401:LEU:HD23	1.73	0.70
1:A:181:VAL:HB	1:A:182:PRO:HD3	1.73	0.69
1:B:385:ARG:HD2	2:B:541:HOH:O	1.91	0.69
1:B:18:GLU:O	1:B:22:VAL:HG12	1.92	0.69
1:B:262:ARG:N	1:B:262:ARG:HD3	2.07	0.69
1:A:119:ARG:NH1	1:A:119:ARG:HG2	2.06	0.69
1:B:176:SER:HB2	1:B:236:LEU:HD11	1.76	0.68
1:A:338:LEU:O	1:A:342:VAL:HG23	1.94	0.67
1:B:169:GLN:HA	2:B:639:HOH:O	1.94	0.67
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.59	0.66
1:B:97:VAL:O	1:B:99:PRO:HD3	1.97	0.65
1:A:219:GLN:HB2	1:A:226:LEU:HD22	1.78	0.64
1:A:21:ARG:HH22	1:A:353:PRO:C	2.01	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ALA:O	1:B:400:ARG:HD3	1.98	0.63
1:A:119:ARG:HH11	1:A:119:ARG:CG	2.12	0.63
1:A:319:ALA:HB3	1:A:342:VAL:HG11	1.81	0.63
1:A:342:VAL:O	1:A:346:THR:HG23	1.99	0.62
1:B:11:TRP:O	1:B:15:VAL:HG22	2.00	0.62
1:A:176:SER:HB2	1:A:236:LEU:HD11	1.81	0.62
1:A:286:ASP:OD2	1:A:364:ARG:HD2	2.00	0.62
1:A:5:ARG:HH21	1:A:402:ALA:CA	2.14	0.61
1:A:96:ARG:HG2	1:A:101:GLU:O	2.00	0.61
1:A:313:TRP:HB3	1:A:360:GLY:HA2	1.82	0.61
1:B:119:ARG:HH21	1:B:119:ARG:H	1.49	0.60
1:B:216:GLN:HG2	1:B:233:GLY:HA3	1.84	0.60
1:A:108:LEU:HD23	1:A:114:PRO:HA	1.84	0.60
1:A:81:LEU:HD12	1:A:81:LEU:O	2.01	0.60
1:A:98:ALA:O	1:A:100:PRO:HD2	2.02	0.60
1:A:321:ILE:HD11	1:A:386:CYS:HA	1.82	0.60
1:A:132:ASN:O	1:A:136:ARG:HG3	2.03	0.59
1:A:392:GLU:HB3	1:B:73:GLU:HG2	1.85	0.59
1:A:21:ARG:HH12	1:A:353:PRO:CA	2.09	0.59
1:B:265:ASP:HB3	1:B:268:LEU:HB3	1.84	0.58
1:A:157:TRP:HE1	1:A:164:GLY:HA3	1.67	0.58
1:A:312:LEU:O	1:A:315:PRO:HD2	2.04	0.58
1:B:305:GLN:NE2	1:B:305:GLN:H	2.01	0.58
1:B:217:HIS:CE1	1:B:229:VAL:HG22	2.38	0.58
1:A:247:GLY:HA3	1:A:315:PRO:HB3	1.86	0.58
1:B:314:TRP:O	1:B:318:GLU:HG2	2.04	0.58
1:A:5:ARG:HH21	1:A:402:ALA:HA	1.68	0.57
1:A:157:TRP:NE1	1:A:164:GLY:HA3	2.19	0.57
1:A:342:VAL:O	1:A:346:THR:CG2	2.52	0.56
1:B:260:SER:HB2	1:B:268:LEU:HD21	1.87	0.56
1:A:385:ARG:HD2	2:A:548:HOH:O	2.05	0.56
1:A:2:GLU:O	1:A:6:GLU:HG3	2.04	0.56
1:B:313:TRP:HB3	1:B:360:GLY:HA2	1.87	0.56
1:B:96:ARG:HD2	1:B:101:GLU:O	2.05	0.56
1:B:327:TYR:CD1	1:B:336:LEU:HB2	2.41	0.56
1:A:89:GLU:OE2	1:A:142:ARG:NH2	2.39	0.56
1:B:176:SER:CB	1:B:236:LEU:HD11	2.36	0.55
1:B:190:GLU:OE1	1:B:258:ARG:HD2	2.05	0.55
1:B:333:PRO:O	1:B:337:ARG:HG3	2.07	0.55
1:B:148:VAL:CG1	1:B:202:ARG:HH22	2.20	0.55
1:B:305:GLN:H	1:B:305:GLN:HE21	1.52	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:VAL:HG23	2:B:532:HOH:O	2.08	0.54
1:B:63:TRP:CZ2	1:B:67:ARG:HD3	2.43	0.54
1:A:350:PHE:CE2	1:A:362:LEU:HD22	2.42	0.54
1:B:94:HIS:HB3	1:B:112:GLY:O	2.08	0.54
1:B:313:TRP:CZ2	1:B:378:LYS:HG3	2.44	0.53
1:B:282:ARG:HG3	1:B:282:ARG:HH21	1.72	0.53
1:A:305:GLN:H	1:A:305:GLN:CD	2.11	0.53
1:B:342:VAL:O	1:B:346:THR:HG23	2.08	0.53
1:A:258:ARG:CA	1:A:325:MET:HE1	2.38	0.53
1:A:79:GLU:CD	1:A:79:GLU:H	2.12	0.53
1:B:219:GLN:HG3	1:B:226:LEU:HD23	1.90	0.52
1:B:33:ARG:NH1	1:B:33:ARG:CG	2.64	0.52
1:A:18:GLU:O	1:A:22:VAL:HG13	2.10	0.52
1:B:47:ARG:HH11	1:B:47:ARG:CG	2.23	0.52
1:B:258:ARG:O	1:B:261:SER:HB3	2.09	0.52
1:A:388:ALA:O	1:A:392:GLU:HG3	2.10	0.52
1:A:305:GLN:NE2	2:A:605:HOH:O	2.42	0.52
1:B:282:ARG:HG3	1:B:282:ARG:NH2	2.24	0.52
1:B:154:ILE:O	1:B:158:VAL:HG13	2.10	0.51
1:B:93:ARG:HH11	1:B:93:ARG:HA	1.74	0.51
1:A:263:SER:O	1:A:265:ASP:N	2.43	0.51
1:A:260:SER:CB	1:A:268:LEU:HD23	2.41	0.51
1:B:350:PHE:CE2	1:B:362:LEU:HD22	2.46	0.51
1:A:119:ARG:HB2	1:A:167:ARG:HD2	1.93	0.51
1:B:1:MET:HB3	1:B:401:LEU:CD2	2.41	0.51
1:B:273:ILE:O	1:B:277:LEU:HB2	2.11	0.51
1:B:34:GLU:HB2	1:B:110:ARG:NH2	2.27	0.50
1:A:55:VAL:HG21	1:A:105:ALA:O	2.11	0.50
1:A:383:VAL:HB	1:A:384:PRO:HD3	1.94	0.50
1:B:342:VAL:O	1:B:346:THR:CG2	2.60	0.50
1:A:153:GLN:NE2	1:A:153:GLN:HA	2.27	0.49
1:A:210:CYS:O	1:A:214:ILE:HG13	2.12	0.49
1:A:277:LEU:HD21	1:A:322:ALA:O	2.13	0.49
1:B:185:LEU:HB3	1:B:210:CYS:SG	2.52	0.49
1:A:192:LEU:HB3	1:A:199:LEU:CD1	2.37	0.49
1:A:166:GLY:O	1:A:167:ARG:HG2	2.13	0.49
1:A:179:MET:O	1:A:182:PRO:HD2	2.13	0.49
1:A:61:GLN:HB2	2:A:509:HOH:O	2.13	0.49
1:A:73:GLU:CG	1:B:392:GLU:HB3	2.41	0.49
1:B:98:ALA:O	1:B:101:GLU:N	2.45	0.48
1:A:190:GLU:OE1	1:A:258:ARG:HD2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:HIS:O	1:A:275:THR:HG23	2.13	0.48
1:A:67:ARG:NH1	1:A:194:GLU:OE1	2.45	0.48
1:B:286:ASP:O	1:B:290:GLY:N	2.44	0.48
1:A:128:THR:HG22	1:A:150:MET:CG	2.43	0.48
1:A:167:ARG:O	1:A:167:ARG:CG	2.60	0.48
1:B:306:LEU:N	1:B:306:LEU:HD23	2.26	0.48
1:A:184:MET:CE	1:A:184:MET:HA	2.43	0.48
1:B:44:ARG:HA	1:B:373:LYS:HG2	1.96	0.48
1:A:94:HIS:HB3	1:A:112:GLY:O	2.14	0.48
1:A:263:SER:O	1:A:264:GLY:C	2.52	0.47
1:B:297:ASP:HB3	1:B:301:LEU:O	2.14	0.47
1:A:5:ARG:NH2	1:A:402:ALA:HB2	2.29	0.47
1:A:118:GLN:HA	1:A:119:ARG:NH2	2.29	0.47
1:A:142:ARG:HB3	2:A:603:HOH:O	2.12	0.47
1:B:5:ARG:HH21	1:B:402:ALA:CB	2.00	0.47
1:A:389:MET:HE3	2:A:599:HOH:O	2.15	0.47
1:A:259:HIS:HA	1:A:262:ARG:NH1	2.29	0.47
1:A:8:LEU:HB2	1:A:398:LEU:HD21	1.97	0.47
1:B:167:ARG:HB2	1:B:167:ARG:NH1	2.30	0.47
2:A:552:HOH:O	1:B:71:LYS:HE2	2.14	0.47
1:A:383:VAL:HB	1:A:384:PRO:CD	2.45	0.46
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.46	0.46
1:B:4:GLU:O	1:B:8:LEU:HG	2.15	0.46
1:A:119:ARG:HG3	1:A:167:ARG:HE	1.80	0.46
1:B:51:ASP:HB2	1:B:110:ARG:HB2	1.98	0.46
1:A:352:ASP:HB2	1:A:359:PHE:CE1	2.51	0.46
1:B:106:PHE:HB2	1:B:118:GLN:HB2	1.97	0.46
1:B:181:VAL:HB	1:B:182:PRO:CD	2.46	0.46
1:B:182:PRO:HB2	1:B:214:ILE:HG13	1.97	0.46
1:A:260:SER:HB2	1:A:268:LEU:HD23	1.97	0.46
1:B:132:ASN:O	1:B:136:ARG:HG3	2.15	0.46
1:A:161:ASP:OD1	1:A:163:SER:HB2	2.16	0.46
1:A:257:LEU:HD13	1:A:272:VAL:HG11	1.97	0.45
1:B:159:ARG:NH1	1:B:209:TRP:CE2	2.84	0.45
1:B:347:PHE:O	1:B:351:ARG:HG3	2.16	0.45
1:B:88:GLY:HA3	1:B:134:LEU:HD11	1.97	0.45
1:A:33:ARG:HB2	1:A:33:ARG:HE	1.53	0.45
1:B:144:GLN:OE1	1:B:144:GLN:HA	2.17	0.45
1:A:197:GLU:OE1	1:B:138:THR:HB	2.17	0.45
1:B:148:VAL:CG1	1:B:202:ARG:NH2	2.80	0.45
1:B:44:ARG:HE	1:B:355:TYR:HD1	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HB3	1:A:325:MET:CE	2.47	0.44
1:B:47:ARG:NH1	1:B:47:ARG:CG	2.80	0.44
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.82	0.44
1:B:218:VAL:CG1	1:B:222:GLY:HA2	2.48	0.44
1:A:96:ARG:HE	1:A:96:ARG:HB2	1.53	0.44
1:B:99:PRO:N	1:B:100:PRO:HD2	2.31	0.44
1:A:138:THR:OG1	1:A:140:GLU:HG3	2.18	0.44
1:A:247:GLY:CA	1:A:315:PRO:HB3	2.48	0.44
1:A:324:LEU:HD23	1:A:390:CYS:HA	2.00	0.44
1:A:106:PHE:HD1	1:A:107:VAL:HG12	1.83	0.44
1:A:124:GLU:O	1:A:128:THR:HG23	2.17	0.44
1:B:159:ARG:NH1	1:B:209:TRP:CD1	2.86	0.44
1:A:265:ASP:C	1:A:265:ASP:OD1	2.54	0.44
1:B:357:GLU:HB3	1:B:373:LYS:HD2	2.00	0.43
1:B:279:LEU:HB3	1:B:280:PRO:CD	2.39	0.43
1:B:242:ARG:HD2	1:B:299:ASP:CG	2.39	0.43
1:B:7:THR:O	1:B:10:ALA:HB3	2.18	0.43
1:A:185:LEU:HB3	1:A:210:CYS:SG	2.59	0.43
1:A:365:GLU:CD	1:A:365:GLU:H	2.22	0.43
1:A:182:PRO:HB2	1:A:214:ILE:HG12	2.00	0.43
1:B:80:LEU:HD12	1:B:80:LEU:H	1.83	0.43
1:A:269:ARG:O	1:A:273:ILE:HD12	2.19	0.43
1:B:166:GLY:O	1:B:167:ARG:HG3	2.19	0.43
1:A:71:LYS:C	1:A:72:LEU:HD12	2.40	0.42
1:B:1:MET:CB	1:B:401:LEU:HD23	2.46	0.42
1:A:250:LEU:HD23	1:A:277:LEU:HA	2.02	0.42
1:A:21:ARG:NH2	1:A:353:PRO:O	2.51	0.42
1:B:313:TRP:CG	1:B:314:TRP:N	2.87	0.42
1:B:257:LEU:HA	1:B:257:LEU:HD12	1.84	0.42
1:A:88:GLY:HA3	1:A:134:LEU:HD11	2.00	0.42
1:B:388:ALA:O	1:B:392:GLU:HG3	2.19	0.42
1:A:183:MET:HA	1:A:214:ILE:HD11	2.02	0.42
1:A:54:TYR:O	1:A:58:GLN:HG2	2.19	0.42
1:B:275:THR:O	1:B:280:PRO:HD3	2.20	0.42
1:B:68:LEU:HD12	1:B:68:LEU:HA	1.90	0.42
1:B:344:GLU:HG3	1:B:348:ARG:NH2	2.35	0.41
1:B:358:TRP:N	1:B:358:TRP:CD1	2.87	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.87	0.41
1:A:212:ARG:O	1:A:216:GLN:HG3	2.20	0.41
1:A:313:TRP:CG	1:A:314:TRP:N	2.88	0.41
1:A:63:TRP:CD1	1:A:133:GLU:HG3	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:HIS:N	1:B:31:HIS:CD2	2.88	0.41
1:B:44:ARG:HB2	1:B:371:THR:O	2.20	0.41
1:A:314:TRP:O	1:A:318:GLU:HG2	2.20	0.41
1:A:399:SER:OG	1:B:74:ARG:HD2	2.19	0.41
1:B:265:ASP:O	1:B:269:ARG:HB2	2.21	0.41
1:B:146:GLU:HA	1:B:146:GLU:OE1	2.20	0.41
1:A:167:ARG:O	1:A:167:ARG:HG2	2.20	0.41
1:A:199:LEU:HD22	1:A:199:LEU:HA	1.96	0.41
1:A:332:ASP:OD1	1:A:332:ASP:C	2.58	0.41
1:B:74:ARG:O	1:B:77:ARG:HD3	2.21	0.41
1:A:259:HIS:CE1	2:A:634:HOH:O	2.74	0.41
1:B:332:ASP:HA	1:B:333:PRO:HD3	1.90	0.41
1:A:119:ARG:NE	1:A:119:ARG:H	2.19	0.40
1:A:319:ALA:CB	1:A:342:VAL:HG11	2.49	0.40
1:B:1:MET:SD	1:B:4:GLU:N	2.94	0.40
1:A:32:ASP:OD2	1:A:110:ARG:HD3	2.22	0.40
1:A:263:SER:C	1:A:265:ASP:N	2.74	0.40
1:A:119:ARG:HB2	1:A:167:ARG:CD	2.50	0.40
1:A:260:SER:HB3	1:A:268:LEU:HD23	2.03	0.40
1:B:151:MET:O	1:B:155:VAL:HG23	2.21	0.40
1:A:217:HIS:CE1	1:A:229:VAL:HG22	2.56	0.40
1:A:88:GLY:HA3	1:A:134:LEU:CD1	2.52	0.40
1:B:51:ASP:HB2	1:B:110:ARG:HD2	2.03	0.40
1:B:92:LEU:HD21	1:B:146:GLU:HG3	2.03	0.40
1:A:119:ARG:HB3	1:A:165:LEU:O	2.21	0.40
1:A:20:ASP:OD2	1:B:399:SER:HB2	2.22	0.40
1:B:129:MET:HG2	1:B:188:LEU:HD23	2.04	0.40
1:B:14:ARG:HG2	1:B:347:PHE:CE2	2.56	0.40
1:B:18:GLU:CD	1:B:351:ARG:HD2	2.42	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	400/402 (100%)	385 (96%)	14 (4%)	1 (0%)	43	39
1	B	400/402 (100%)	368 (92%)	30 (8%)	2 (0%)	31	25
All	All	800/804 (100%)	753 (94%)	44 (6%)	3 (0%)	36	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLY
1	B	168	PRO
1	B	100	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	334/334 (100%)	282 (84%)	52 (16%)	3	1
1	B	334/334 (100%)	293 (88%)	41 (12%)	5	3
All	All	668/668 (100%)	575 (86%)	93 (14%)	4	2

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLU
1	A	13	GLU
1	A	22	VAL
1	A	27	LEU
1	A	33	ARG
1	A	44	ARG
1	A	47	ARG
1	A	68	LEU
1	A	74	ARG
1	A	79	GLU
1	A	81	LEU
1	A	93	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	ARG
1	A	107	VAL
1	A	110	ARG
1	A	119	ARG
1	A	123	SER
1	A	128	THR
1	A	142	ARG
1	A	153	GLN
1	A	159	ARG
1	A	161	ASP
1	A	167	ARG
1	A	169	GLN
1	A	170	LEU
1	A	174	VAL
1	A	195	GLU
1	A	198	GLU
1	A	199	LEU
1	A	202	ARG
1	A	212	ARG
1	A	226	LEU
1	A	248	HIS
1	A	257	LEU
1	A	258	ARG
1	A	260	SER
1	A	262	ARG
1	A	275	THR
1	A	282	ARG
1	A	301	LEU
1	A	304	THR
1	A	305	GLN
1	A	313	TRP
1	A	346	THR
1	A	357	GLU
1	A	362	LEU
1	A	364	ARG
1	A	385	ARG
1	A	386	CYS
1	A	399	SER
1	A	401	LEU
1	B	1	MET
1	B	3	LYS
1	B	5	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	7	THR
1	B	13	GLU
1	B	21	ARG
1	B	22	VAL
1	B	33	ARG
1	B	68	LEU
1	B	72	LEU
1	B	79	GLU
1	B	93	ARG
1	B	97	VAL
1	B	107	VAL
1	B	119	ARG
1	B	123	SER
1	B	165	LEU
1	B	167	ARG
1	B	170	LEU
1	B	178	SER
1	B	197	GLU
1	B	202	ARG
1	B	216	GLN
1	B	226	LEU
1	B	248	HIS
1	B	257	LEU
1	B	258	ARG
1	B	260	SER
1	B	262	ARG
1	B	263	SER
1	B	268	LEU
1	B	269	ARG
1	B	282	ARG
1	B	301	LEU
1	B	304	THR
1	B	305	GLN
1	B	313	TRP
1	B	346	THR
1	B	357	GLU
1	B	386	CYS
1	B	401	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	223	GLN
1	A	259	HIS
1	A	305	GLN
1	B	305	GLN

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 carbohydrates 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.