



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:41 PM UTC

PDB ID : 1FP3 / pdb_00001fp3
Title : CRYSTAL STRUCTURE OF N-ACYL-D-GLUCOSAMINE 2-EPIMERASE
FROM PORCINE KIDNEY
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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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

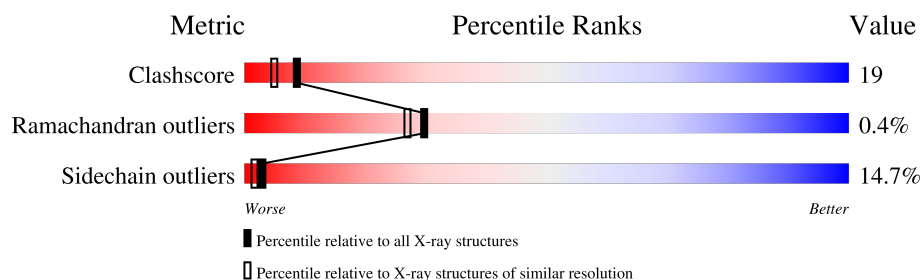
1 Overall quality at a glance

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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

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.

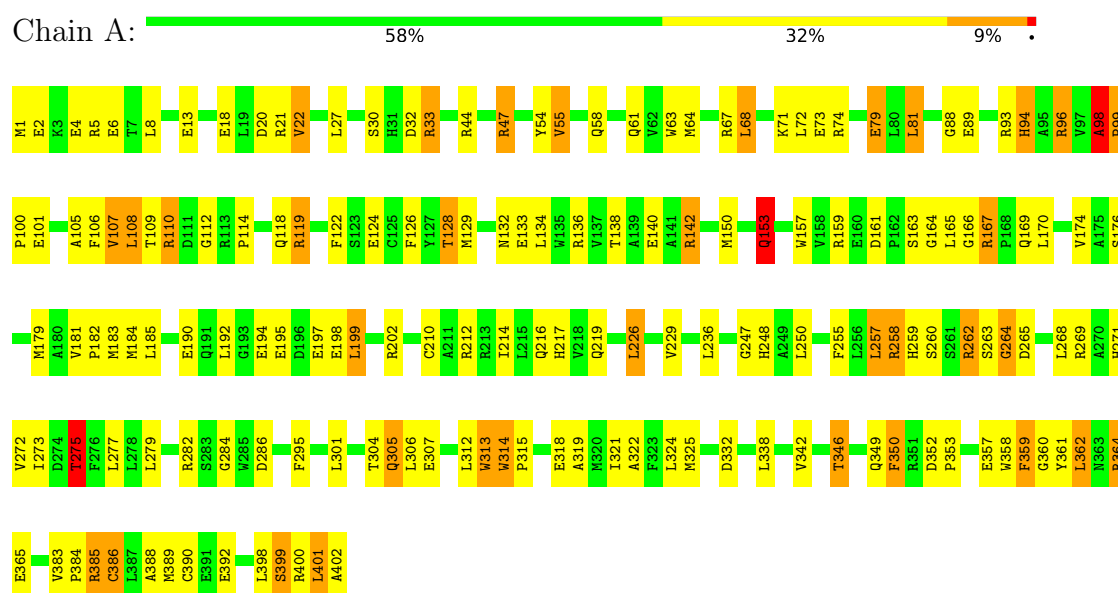
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	67	Total	O	0	0
			67	67		

3 Residue-property plots [i](#)

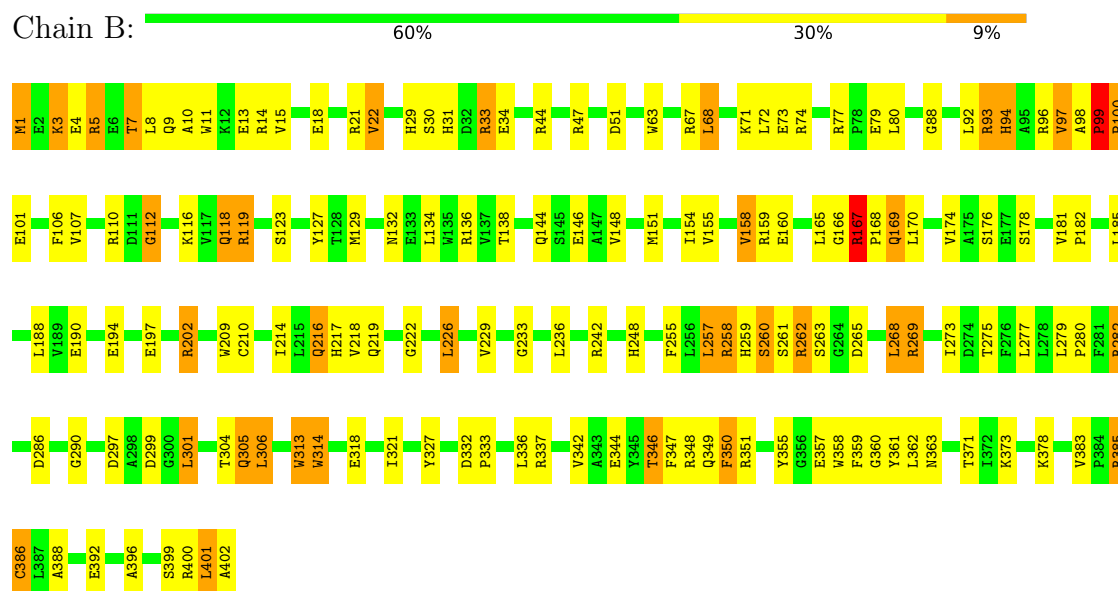
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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



• 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

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	0.48	0/3354	0.97	20/4527 (0.4%)
1	B	0.47	0/3354	0.96	16/4527 (0.4%)
All	All	0.47	0/6708	0.97	36/9054 (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	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	PHE	N-CA-C	-8.69	99.06	110.53
1	B	30	SER	N-CA-C	8.00	122.81	112.89
1	A	122	PHE	N-CA-C	7.99	119.98	111.28
1	B	359	PHE	N-CA-C	-7.91	98.78	110.48
1	A	255	PHE	N-CA-C	-7.56	102.97	111.14
1	B	127	TYR	N-CA-C	-7.50	103.10	111.28
1	A	94	HIS	N-CA-C	7.18	122.34	113.50
1	A	275	THR	N-CA-C	6.86	120.88	112.23
1	A	30	SER	N-CA-C	6.63	121.39	113.16
1	B	99	PRO	N-CA-C	6.44	118.56	110.70
1	A	313	TRP	N-CA-C	6.37	118.22	111.28
1	B	255	PHE	N-CA-C	-6.34	104.45	111.36
1	A	99	PRO	N-CA-C	6.19	118.25	110.70
1	A	361	TYR	N-CA-C	6.10	118.35	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	PHE	N-CA-C	6.07	120.76	113.23
1	A	153	GLN	N-CA-C	-5.98	104.68	111.14
1	B	361	TYR	N-CA-C	5.98	118.15	108.41
1	A	349	GLN	N-CA-C	5.96	120.74	112.45
1	B	112	GLY	N-CA-C	5.91	123.77	115.43
1	B	167	ARG	CA-C-N	5.85	127.15	119.84
1	B	167	ARG	C-N-CA	5.85	127.15	119.84
1	A	350	PHE	N-CA-C	5.77	120.46	112.90
1	B	313	TRP	N-CA-C	5.69	117.16	111.07
1	A	55	VAL	N-CA-C	5.66	117.07	110.62
1	B	29	HIS	N-CA-C	5.64	120.82	113.88
1	A	109	THR	N-CA-C	-5.64	103.47	110.41
1	A	98	ALA	CA-C-N	5.55	126.10	120.38
1	A	98	ALA	C-N-CA	5.55	126.10	120.38
1	B	94	HIS	N-CA-C	5.50	121.54	114.56
1	A	314	TRP	N-CA-C	5.30	121.53	109.81
1	A	307	GLU	N-CA-C	5.25	119.32	113.02
1	A	401	LEU	N-CA-C	-5.23	107.07	113.50
1	B	314	TRP	N-CA-C	5.20	121.29	109.81
1	A	284	GLY	N-CA-C	5.19	120.32	113.37
1	B	349	GLN	N-CA-C	5.07	119.50	112.45
1	B	363	ASN	N-CA-C	-5.02	103.42	110.35

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 ⓘ

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	131	0
1	B	3265	0	3154	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	78	0	0	7	0
2	B	67	0	0	3	0
All	All	6675	0	6308	241	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 19.

All (241) 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:HG2	1:B:33:ARG:HH11	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:257:LEU:HB3	1:A:325:MET:HE2	1.57	0.87
1:A:21:ARG:NH1	1:A:353:PRO:HA	1.91	0.85
1:B:33:ARG:HG2	1:B:33:ARG:NH1	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: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:HG2	1:A:119:ARG:HH11	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:HD3	1:B:262:ARG:N	2.07	0.69
1:A:119:ARG:HG2	1:A:119:ARG:NH1	2.06	0.69
1:A:21:ARG:HH22	1:A:353:PRO:C	2.01	0.68
1:B:176:SER:HB2	1:B:236:LEU:HD11	1.76	0.68
1:A:258:ARG:CA	1:A:325:MET:HE1	2.24	0.67
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:HG3	1:B:47:ARG:HH11	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

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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:H	1:B:119:ARG:HH21	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:A:258:ARG:HA	1:A:325:MET:HE1	1.83	0.59
1:A:184:MET:HE3	1:A:184:MET:HA	1.84	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:H	1:B:305:GLN:NE2	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:305:GLN:CD	1:A:305:GLN:H	2.11	0.57
1:A:79:GLU:CD	1:A:79:GLU:H	2.12	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:A:385:ARG:HD2	2:A:548:HOH:O	2.05	0.56
1:B:260:SER:HB2	1:B:268:LEU:HD21	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HH21	1:B:282:ARG:HG3	1.72	0.53
1:B:342:VAL:O	1:B:346:THR:HG23	2.08	0.53
1:B:33:ARG:NH1	1:B:33:ARG:CG	2.64	0.52
1:B:219:GLN:HG3	1:B:226:LEU:HD23	1.90	0.52
1:A:263:SER:O	1:A:264:GLY:C	2.52	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:64:MET:HE3	1:A:64:MET:HA	1.91	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:93:ARG:HA	1:B:93:ARG:HH11	1.74	0.51
1:B:154:ILE:O	1:B:158:VAL:HG13	2.10	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:HA	1:A:153:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:ARG:NH1	1:A:194:GLU:OE1	2.45	0.48
1:A:190:GLU:OE1	1:A:258:ARG:HD2	2.13	0.48
1:A:265:ASP:OD1	1:A:265:ASP:C	2.54	0.48
1:A:271:HIS:O	1:A:275:THR:HG23	2.13	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:CG	1:A:167:ARG:O	2.60	0.48
1:B:306:LEU:N	1:B:306:LEU:HD23	2.26	0.48
1:B:242:ARG:HD2	1:B:299:ASP:CG	2.39	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:184:MET:HA	1:A:184:MET:CE	2.43	0.48
1:A:365:GLU:H	1:A:365:GLU:CD	2.22	0.48
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:71:LYS:C	1:A:72:LEU:HD12	2.40	0.47
1:A:389:MET:HE3	2:A:599:HOH:O	2.15	0.47
1:A:8:LEU:HB2	1:A:398:LEU:HD21	1.97	0.47
1:A:259:HIS:HA	1:A:262:ARG:NH1	2.29	0.47
2:A:552:HOH:O	1:B:71:LYS:HE2	2.14	0.47
1:B:167:ARG:HB2	1:B:167:ARG:NH1	2.30	0.47
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.46	0.46
1:A:383:VAL:HB	1:A:384:PRO:CD	2.45	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:126:PHE:CD1	1:A:129:MET:HE3	2.51	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:332:ASP:OD1	1:A:332:ASP:C	2.58	0.46
1:A:257:LEU:HD13	1:A:272:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:NH1	1:B:209:TRP:CE2	2.84	0.45
1:B:88:GLY:HA3	1:B:134:LEU:HD11	1.97	0.45
1:B:347:PHE:O	1:B:351:ARG:HG3	2.16	0.45
1:A:33:ARG:HE	1:A:33:ARG:HB2	1.53	0.45
1:B:18:GLU:CD	1:B:351:ARG:HD2	2.42	0.45
1:B:144:GLN:HA	1:B:144:GLN:OE1	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
1:B:47:ARG:CG	1:B:47:ARG:NH1	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:B:357:GLU:C	1:B:358:TRP:HD1	2.25	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:A:258:ARG:N	1:A:325:MET:HE1	2.33	0.44
1:B:1:MET:SD	1:B:1:MET:C	3.00	0.44
1:B:159:ARG:NH1	1:B:209:TRP:CD1	2.86	0.44
1:A:163:SER:C	1:A:165:LEU:H	2.24	0.44
1:A:263:SER:C	1:A:265:ASP:N	2.74	0.43
1:B:357:GLU:HB3	1:B:373:LYS:HD2	2.00	0.43
1:A:357:GLU:C	1:A:358:TRP:HD1	2.27	0.43
1:B:1:MET:HE1	1:B:3:LYS:HB2	2.00	0.43
1:B:279:LEU:HB3	1:B:280:PRO:CD	2.39	0.43
1:A:64:MET:HE2	1:A:68:LEU:HD13	2.00	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: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: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:A:163:SER:C	1:A:165:LEU:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LEU:HD12	1:B:257:LEU:HA	1.84	0.42
1:A:88:GLY:HA3	1:A:134:LEU:HD11	2.00	0.42
1:A:365:GLU:CD	1:A:365:GLU:N	2.78	0.42
1:B:388:ALA:O	1:B:392:GLU:HG3	2.19	0.42
1:A:54:TYR:O	1:A:58:GLN:HG2	2.19	0.42
1:A:183:MET:HA	1:A:214:ILE:HD11	2.02	0.42
1:B:68:LEU:HD12	1:B:68:LEU:HA	1.90	0.42
1:B:275:THR:O	1:B:280:PRO:HD3	2.20	0.42
1:B:344:GLU:HG3	1:B:348:ARG:NH2	2.35	0.41
1:B:358:TRP:CD1	1:B:358:TRP:N	2.87	0.41
1:A:179:MET:HE3	1:A:217:HIS:CB	2.51	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.87	0.41
1:B:259:HIS:C	1:B:261:SER:H	2.28	0.41
1:A:63:TRP:CD1	1:A:133:GLU:HG3	2.54	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:B:31:HIS:CD2	1:B:31:HIS:N	2.88	0.41
1:A:98:ALA:C	1:A:100:PRO:HD2	2.45	0.41
1:B:44:ARG:HB2	1:B:371:THR:O	2.20	0.41
1:B:159:ARG:HH12	1:B:209:TRP:CD1	2.38	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:OE1	1:B:146:GLU:HA	2.20	0.41
1:A:167:ARG:HG2	1:A:167:ARG:O	2.20	0.41
1:A:199:LEU:HD22	1:A:199:LEU:HA	1.96	0.41
1:A:184:MET:HE3	1:A:184:MET:CA	2.49	0.41
1:A:259:HIS:CE1	2:A:634:HOH:O	2.74	0.41
1:B:74:ARG:O	1:B:77:ARG:HD3	2.21	0.41
1:B:332:ASP:HA	1:B:333:PRO:HD3	1.90	0.41
1:A:119:ARG:H	1:A:119:ARG:NE	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: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:129:MET:HE2	1:B:129:MET:HB3	1.89	0.40
1:B:151:MET:O	1:B:155:VAL:HG23	2.21	0.40
1:A:88:GLY:HA3	1:A:134:LEU:CD1	2.52	0.40
1:A:217:HIS:CE1	1:A:229:VAL:HG22	2.56	0.40
1:B:51:ASP:HB2	1:B:110:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD21	1:B:146:GLU:HG3	2.03	0.40
1:A:20:ASP:OD2	1:B:399:SER:HB2	2.22	0.40
1:A:119:ARG:HB3	1:A:165:LEU:O	2.21	0.40
1:B:14:ARG:HG2	1:B:347:PHE:CE2	2.56	0.40
1:B:129:MET:HG2	1:B:188:LEU:HD23	2.04	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	A	400/402 (100%)	385 (96%)	14 (4%)	1 (0%)	36	35
1	B	400/402 (100%)	368 (92%)	30 (8%)	2 (0%)	24	21
All	All	800/804 (100%)	753 (94%)	44 (6%)	3 (0%)	30	27

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 [i](#)

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%)	284 (85%)	50 (15%)	3	1
1	B	334/334 (100%)	286 (86%)	48 (14%)	3	2
All	All	668/668 (100%)	570 (85%)	98 (15%)	3	2

All (98) 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
1	A	96	ARG
1	A	107	VAL
1	A	108	LEU
1	A	110	ARG
1	A	119	ARG
1	A	128	THR
1	A	142	ARG
1	A	153	GLN
1	A	159	ARG
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	226	LEU
1	A	248	HIS
1	A	257	LEU
1	A	258	ARG
1	A	262	ARG

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Mol	Chain	Res	Type
1	A	275	THR
1	A	279	LEU
1	A	282	ARG
1	A	301	LEU
1	A	304	THR
1	A	305	GLN
1	A	306	LEU
1	A	346	THR
1	A	362	LEU
1	A	364	ARG
1	A	385	ARG
1	A	386	CYS
1	A	399	SER
1	A	400	ARG
1	A	401	LEU
1	B	1	MET
1	B	3	LYS
1	B	5	ARG
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	116	LYS
1	B	118	GLN
1	B	119	ARG
1	B	123	SER
1	B	158	VAL
1	B	160	GLU
1	B	165	LEU
1	B	167	ARG
1	B	169	GLN
1	B	170	LEU
1	B	174	VAL
1	B	178	SER
1	B	194	GLU

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Mol	Chain	Res	Type
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	306	LEU
1	B	346	THR
1	B	385	ARG
1	B	386	CYS
1	B	401	LEU

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	153	GLN
1	A	169	GLN
1	A	216	GLN
1	A	223	GLN
1	A	228	ASN
1	A	259	HIS
1	A	296	GLN
1	A	305	GLN
1	A	341	GLN
1	B	29	HIS
1	B	259	HIS
1	B	271	HIS
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 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

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.