



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:34 AM GMT

PDB ID : 2DKA
Title : Crystal structure of N-acetylglucosamine-phosphate mutase, a member of the alpha-D-phosphohexomutase superfamily, in the apo-form
Authors : Nishitani, Y.; Maruyama, D.; Nonaka, T.; Kita, A.; Fukami, T.A.; Mio, T.; Yamada-Okabe, H.; Yamada-Okabe, T.; Miki, K.
Deposited on : 2006-04-07
Resolution : 1.93 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

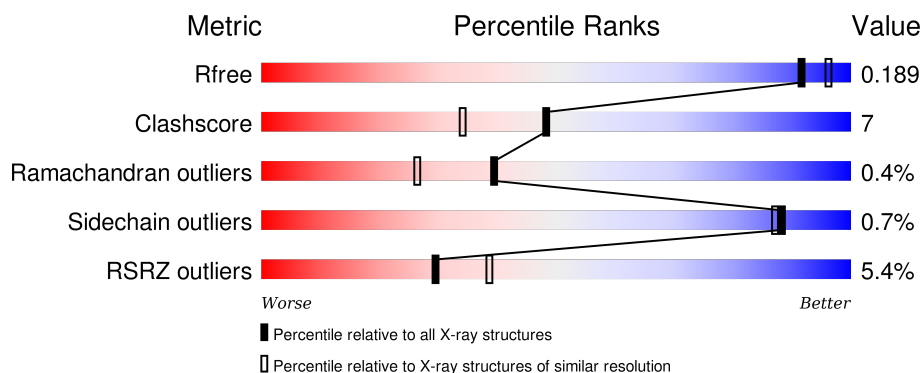
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	544	
1	B	544	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8413 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 Phosphoacetylglucosamine mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4027	2568	663	788	8			
1	B	461	Total	C	N	O	S	0	0	0
			3584	2290	586	701	7			

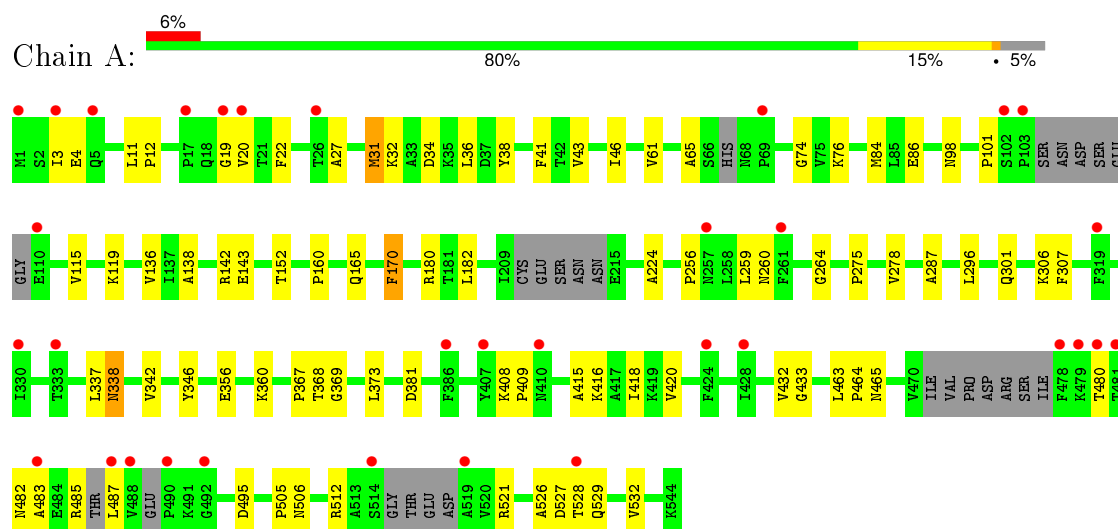
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	408	Total	O	0	0
			408	408		
2	B	394	Total	O	0	0
			394	394		

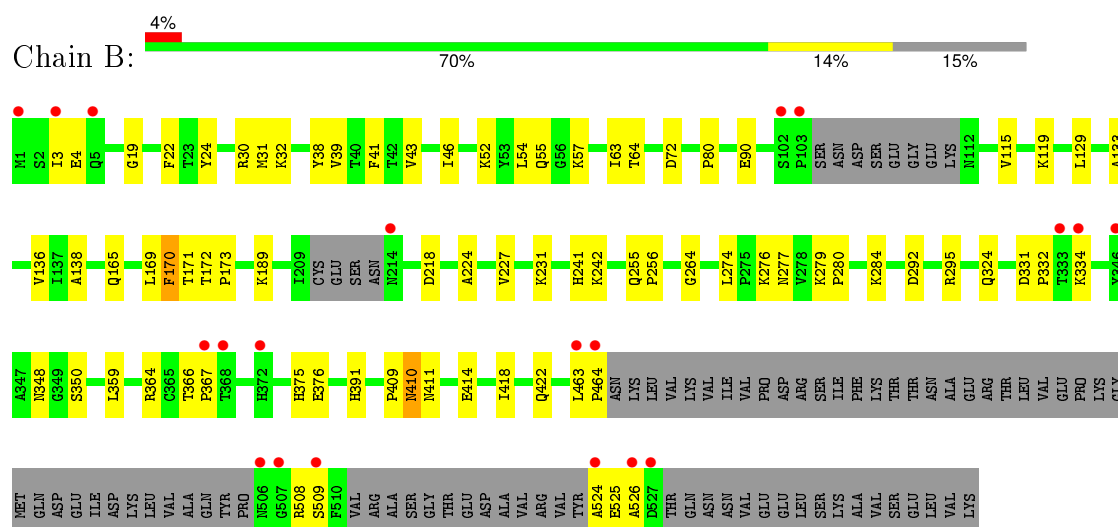
3 Residue-property plots [i](#)

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: Phosphoacetylglucosamine mutase



• Molecule 1: Phosphoacetylglucosamine mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.17Å 130.22Å 77.96Å 90.00° 106.68° 90.00°	Depositor
Resolution (Å)	29.56 – 1.93 29.56 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.56-1.93) 99.7 (29.56-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 1.93Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.222 0.193 , 0.189	Depositor DCC
R_{free} test set	4285 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 85910 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8413	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.31	0/4104	0.56	0/5572
1	B	0.31	0/3659	0.57	0/4973
All	All	0.31	0/7763	0.57	0/10545

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4027	0	3949	63	0
1	B	3584	0	3519	48	0
2	A	408	0	0	8	0
2	B	394	0	0	2	0
All	All	8413	0	7468	110	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 7.

All (110) 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:A:338:ASN:HD21	1:A:381:ASP:H	1.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:HA	1:A:76:LYS:HE2	1.56	0.87
1:A:338:ASN:ND2	1:A:381:ASP:H	1.82	0.77
1:A:338:ASN:HD22	1:A:338:ASN:C	1.87	0.76
1:B:57:LYS:HE3	1:B:80:PRO:HG2	1.69	0.75
1:A:482:ASN:ND2	1:A:485:ARG:HH21	1.88	0.72
1:A:482:ASN:HD21	1:A:485:ARG:HH21	1.36	0.71
1:B:32:LYS:HD3	1:B:72:ASP:OD1	1.94	0.67
1:A:22:PHE:H	1:A:98:ASN:HD21	1.46	0.64
1:A:138:ALA:HB1	1:A:170:PHE:HB2	1.80	0.64
1:B:136:VAL:HG12	1:B:165:GLN:HB3	1.81	0.62
1:A:409:PRO:HG3	1:A:415:ALA:HA	1.82	0.61
1:B:189:LYS:HE3	2:B:582:HOH:O	2.01	0.60
1:A:464:PRO:HD2	1:A:526:ALA:O	2.03	0.59
1:B:54:LEU:HB3	1:B:57:LYS:HE2	1.86	0.57
1:B:464:PRO:HD2	1:B:526:ALA:O	2.05	0.57
1:A:11:LEU:HD11	1:A:101:PRO:HB3	1.87	0.57
1:A:76:LYS:HD3	2:A:685:HOH:O	2.06	0.55
1:A:3:ILE:HD12	1:A:160:PRO:HD3	1.88	0.55
1:A:65:ALA:HB3	1:A:142:ARG:CZ	2.36	0.55
1:B:169:LEU:HG	1:B:227:VAL:HG23	1.87	0.55
1:A:36:LEU:HD21	1:A:74:GLY:HA2	1.89	0.54
1:B:22:PHE:CD2	1:B:39:VAL:HG21	2.42	0.54
1:A:527:ASP:OD2	1:A:528:THR:HG23	2.08	0.54
1:A:84:MET:HE1	2:A:951:HOH:O	2.08	0.53
1:B:409:PRO:HB3	1:B:414:GLU:HB3	1.90	0.53
1:A:180:ARG:NE	2:A:874:HOH:O	2.42	0.53
1:A:342:VAL:HG12	1:A:373:LEU:HD23	1.91	0.53
1:B:138:ALA:HB1	1:B:170:PHE:HB2	1.91	0.52
1:A:367:PRO:HG3	1:A:483:ALA:HA	1.89	0.52
1:A:306:LYS:HD2	1:A:307:PHE:N	2.24	0.52
1:A:259:LEU:CD1	1:A:260:ASN:ND2	2.73	0.52
1:A:180:ARG:HH11	1:A:180:ARG:HG3	1.76	0.51
1:B:24:TYR:CD2	1:B:90:GLU:HG2	2.45	0.51
1:B:418:ILE:O	1:B:422:GLN:HG3	2.11	0.51
1:B:115:VAL:HG22	1:B:119:LYS:HE3	1.92	0.50
1:B:218:ASP:OD2	1:B:284:LYS:NZ	2.44	0.50
1:A:11:LEU:HD11	1:A:101:PRO:CB	2.42	0.50
1:A:415:ALA:O	1:A:418:ILE:HG22	2.10	0.50
1:A:337:LEU:HA	1:A:381:ASP:OD1	2.12	0.49
1:A:306:LYS:HD2	1:A:307:PHE:H	1.77	0.49
1:A:338:ASN:HD21	1:A:381:ASP:N	2.03	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLN:O	1:A:532:VAL:HG12	2.11	0.49
1:A:306:LYS:HE3	1:A:307:PHE:O	2.13	0.48
1:B:31:MET:HB2	2:B:823:HOH:O	2.13	0.48
1:A:480:THR:HG22	1:A:487:LEU:HD13	1.95	0.48
1:B:410:ASN:HD22	1:B:411:ASN:N	2.11	0.48
1:A:256:PRO:HA	2:A:803:HOH:O	2.13	0.48
1:B:331:ASP:CG	1:B:334:LYS:HD3	2.33	0.47
1:A:11:LEU:HB3	1:A:12:PRO:HD3	1.97	0.47
1:B:274:LEU:CD1	1:B:280:PRO:HB3	2.44	0.47
1:A:86:GLU:OE1	1:B:375:HIS:HE1	1.97	0.47
1:A:275:PRO:HG2	1:A:278:VAL:CG2	2.45	0.47
1:A:4:GLU:HG3	1:A:115:VAL:HG21	1.96	0.47
1:A:32:LYS:HB3	1:A:34:ASP:OD1	2.14	0.47
1:A:115:VAL:O	1:A:119:LYS:HG3	2.15	0.47
1:B:63:ILE:O	1:B:64:THR:HB	2.14	0.47
1:A:76:LYS:NZ	2:A:683:HOH:O	2.47	0.46
1:A:338:ASN:ND2	1:A:338:ASN:C	2.61	0.46
1:B:22:PHE:CE2	1:B:39:VAL:HG21	2.50	0.46
1:A:505:PRO:O	1:A:506:ASN:HB2	2.16	0.45
1:A:38:TYR:O	1:A:41:PHE:HB3	2.16	0.45
1:A:416:LYS:O	1:A:420:VAL:HG23	2.16	0.45
1:A:43:VAL:O	1:A:46:ILE:HG22	2.16	0.45
1:B:410:ASN:C	1:B:410:ASN:HD22	2.19	0.45
1:B:276:LYS:O	1:B:277:ASN:HB2	2.17	0.45
1:A:287:ALA:HB1	1:A:296:LEU:HD11	1.98	0.45
1:A:136:VAL:HG12	1:A:165:GLN:HB3	1.98	0.45
1:B:350:SER:OG	1:B:463:LEU:HG	2.18	0.44
1:B:171:THR:HG23	1:B:231:LYS:HG3	1.99	0.44
1:B:43:VAL:O	1:B:46:ILE:HG22	2.17	0.44
1:B:366:THR:HB	1:B:367:PRO:HD2	1.99	0.44
1:A:3:ILE:HG23	1:A:4:GLU:N	2.33	0.44
1:B:364:ARG:HG3	1:B:364:ARG:HH11	1.82	0.43
1:A:224:ALA:HB2	1:A:264:GLY:HA2	1.99	0.43
1:B:255:GLN:HA	1:B:256:PRO:HD2	1.75	0.43
1:B:324:GLN:NE2	1:B:359:LEU:HA	2.33	0.43
1:B:348:ASN:ND2	1:B:350:SER:H	2.16	0.43
2:A:627:HOH:O	1:B:55:GLN:HG2	2.19	0.43
1:A:301:GLN:NE2	2:A:832:HOH:O	2.47	0.42
1:B:64:THR:OG1	1:B:292:ASP:OD1	2.32	0.42
1:A:432:VAL:HG22	1:A:433:GLY:N	2.34	0.42
1:B:224:ALA:HB2	1:B:264:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:THR:HB	1:B:173:PRO:HD3	2.02	0.42
1:A:76:LYS:HB3	1:A:76:LYS:NZ	2.35	0.42
1:A:275:PRO:HG2	1:A:278:VAL:HG23	2.02	0.42
1:B:508:ARG:O	1:B:525:GLU:O	2.38	0.42
1:B:509:SER:HA	1:B:524:ALA:HB1	2.02	0.42
1:A:346:TYR:OH	1:A:512:ARG:HD3	2.20	0.42
2:A:626:HOH:O	1:B:57:LYS:HE2	2.19	0.42
1:B:241:HIS:CE1	1:B:242:LYS:HG3	2.54	0.41
1:B:38:TYR:O	1:B:41:PHE:HB3	2.20	0.41
1:B:295:ARG:HG2	1:B:391:HIS:HB2	2.02	0.41
1:A:31:MET:CG	1:A:36:LEU:HD13	2.50	0.41
1:A:465:ASN:HA	1:A:532:VAL:HG21	2.02	0.41
1:A:368:THR:HG22	1:A:369:GLY:N	2.35	0.41
1:A:408:LYS:HA	1:A:409:PRO:HD2	1.96	0.41
1:B:30:ARG:O	1:B:31:MET:HB3	2.21	0.41
1:B:52:LYS:HD3	1:B:129:LEU:HA	2.03	0.41
1:B:52:LYS:HG3	1:B:133:ALA:HB2	2.03	0.41
1:A:61:VAL:HG11	1:A:152:THR:HG21	2.02	0.41
1:A:259:LEU:HD13	1:A:260:ASN:ND2	2.36	0.41
1:B:331:ASP:HA	1:B:332:PRO:HD2	1.97	0.41
1:B:279:LYS:HA	1:B:280:PRO:HD2	1.87	0.41
1:A:136:VAL:HG11	1:A:182:LEU:CD1	2.51	0.41
1:B:364:ARG:HG3	1:B:376:GLU:OE1	2.20	0.40
1:A:463:LEU:O	1:A:464:PRO:C	2.58	0.40
1:B:3:ILE:HG23	1:B:4:GLU:N	2.36	0.40
1:A:356:GLU:O	1:A:360:LYS:HA	2.21	0.40
1:A:521:ARG:HH11	1:A:521:ARG:HG2	1.84	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	503/544 (92%)	487 (97%)	13 (3%)	3 (1%)	30	16
1	B	451/544 (83%)	432 (96%)	18 (4%)	1 (0%)	52	42
All	All	954/1088 (88%)	919 (96%)	31 (3%)	4 (0%)	39	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	19	GLY
1	A	31	MET
1	B	19	GLY

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	442/480 (92%)	438 (99%)	4 (1%)	84	82
1	B	396/480 (82%)	394 (100%)	2 (0%)	92	92
All	All	838/960 (87%)	832 (99%)	6 (1%)	88	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	170	PHE
1	A	338	ASN
1	A	495	ASP
1	B	170	PHE
1	B	410	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	120	ASN
1	A	277	ASN
1	A	282	ASN
1	A	301	GLN
1	A	324	GLN
1	A	325	GLN
1	A	338	ASN
1	A	343	GLN
1	A	482	ASN
1	A	494	GLN
1	A	506	ASN
1	A	529	GLN
1	A	531	ASN
1	B	5	GLN
1	B	204	GLN
1	B	255	GLN
1	B	271	ASN
1	B	277	ASN
1	B	301	GLN
1	B	325	GLN
1	B	343	GLN
1	B	348	ASN
1	B	375	HIS
1	B	410	ASN
1	B	413	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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, 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	519/544 (95%)	0.21	33 (6%)	23 31	12, 25, 50, 60	0
1	B	461/544 (84%)	0.14	20 (4%)	39 48	12, 23, 47, 60	0
All	All	980/1088 (90%)	0.18	53 (5%)	29 39	12, 24, 50, 60	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	463	LEU	6.7
1	B	346	TYR	6.3
1	B	509	SER	6.1
1	A	488	VAL	5.6
1	A	478	PHE	5.2
1	A	480	THR	4.9
1	B	526	ALA	4.7
1	B	368	THR	4.5
1	A	490	PRO	4.5
1	A	487	LEU	4.4
1	B	527	ASP	4.0
1	A	479	LYS	3.7
1	A	103	PRO	3.7
1	B	367	PRO	3.7
1	A	1	MET	3.5
1	B	214	ASN	3.5
1	A	407	TYR	3.4
1	B	103	PRO	3.3
1	A	110	GLU	3.2
1	B	506	ASN	3.2
1	B	102	SER	3.2
1	A	481	THR	3.1
1	A	330	ILE	3.1
1	A	5	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	492	GLY	3.0
1	B	1	MET	3.0
1	B	507	GLY	2.9
1	B	372	HIS	2.8
1	B	464	PRO	2.7
1	A	424	PHE	2.7
1	A	514	SER	2.6
1	B	524	ALA	2.6
1	B	5	GLN	2.6
1	A	17	PRO	2.5
1	A	257	ASN	2.5
1	A	19	GLY	2.5
1	A	102	SER	2.4
1	A	519	ALA	2.4
1	A	410	ASN	2.3
1	A	333	THR	2.3
1	A	69	PRO	2.3
1	B	334	LYS	2.2
1	A	528	THR	2.2
1	A	483	ALA	2.2
1	B	333	THR	2.2
1	A	428	ILE	2.2
1	A	386	PHE	2.1
1	A	3	ILE	2.1
1	A	26	THR	2.1
1	A	20	VAL	2.1
1	A	261	PHE	2.1
1	B	3	ILE	2.1
1	A	319	PHE	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 [i](#)

There are no such residues in this entry.