Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:00 PM EDT

PDB ID	:	6HKI
Title	:	Crystal structure of surface entropy mutant of human O-GlcNAc hydrolase
Authors	:	Males, A.; Davies, G.J.
Deposited on	:	2018-09-06
Resolution	:	3.30 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:

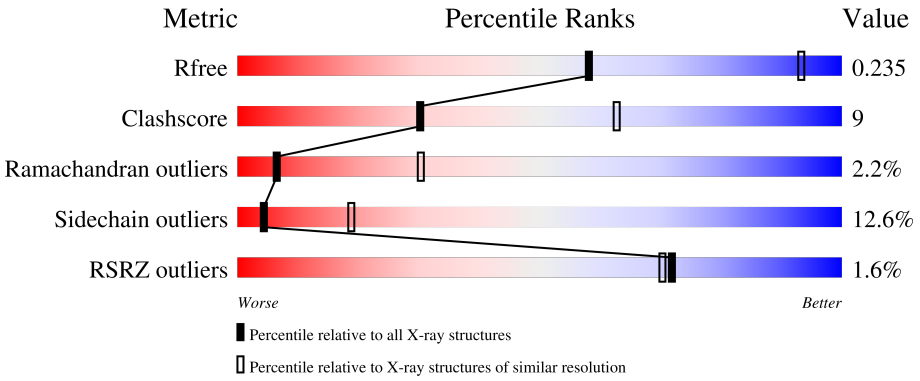
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	916	% 39% 11% • 47%
1	B	916	% 37% 14% • 47%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7880 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 Protein O-GlcNAcase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	2	0
			3965	2562	657	721	25			
1	B	486	Total	C	N	O	S	0	0	0
			3914	2531	650	708	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	602	ALA	GLU	engineered mutation	UNP O60502
A	605	ALA	GLU	engineered mutation	UNP O60502
B	602	ALA	GLU	engineered mutation	UNP O60502
B	605	ALA	GLU	engineered mutation	UNP O60502

- Molecule 2 is water.

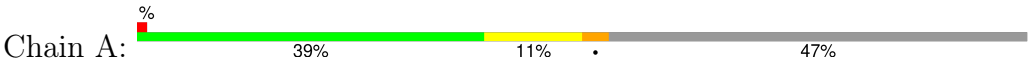
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		

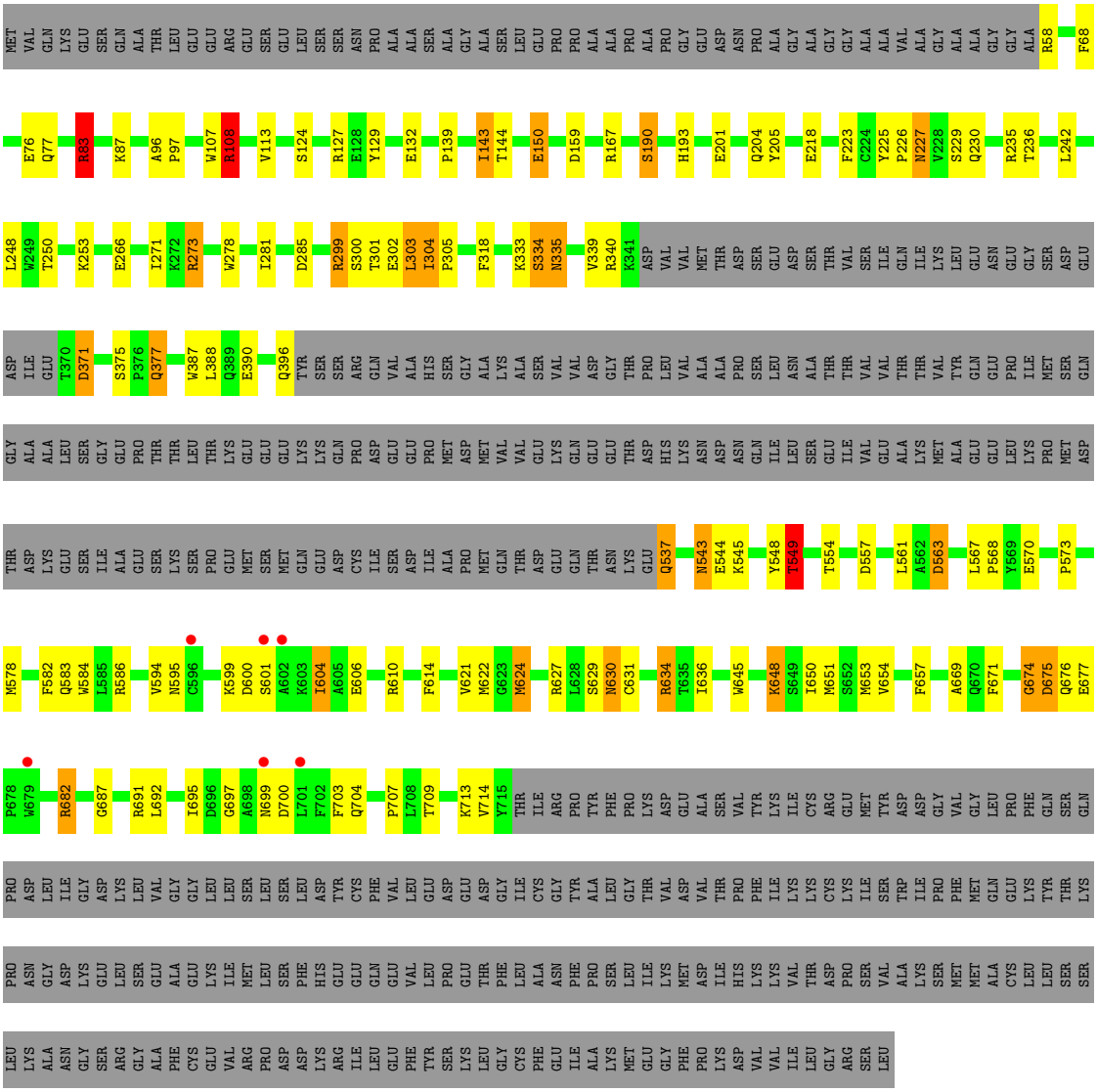
3 Residue-property plots (i)

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 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: Protein O-GlcNAcase

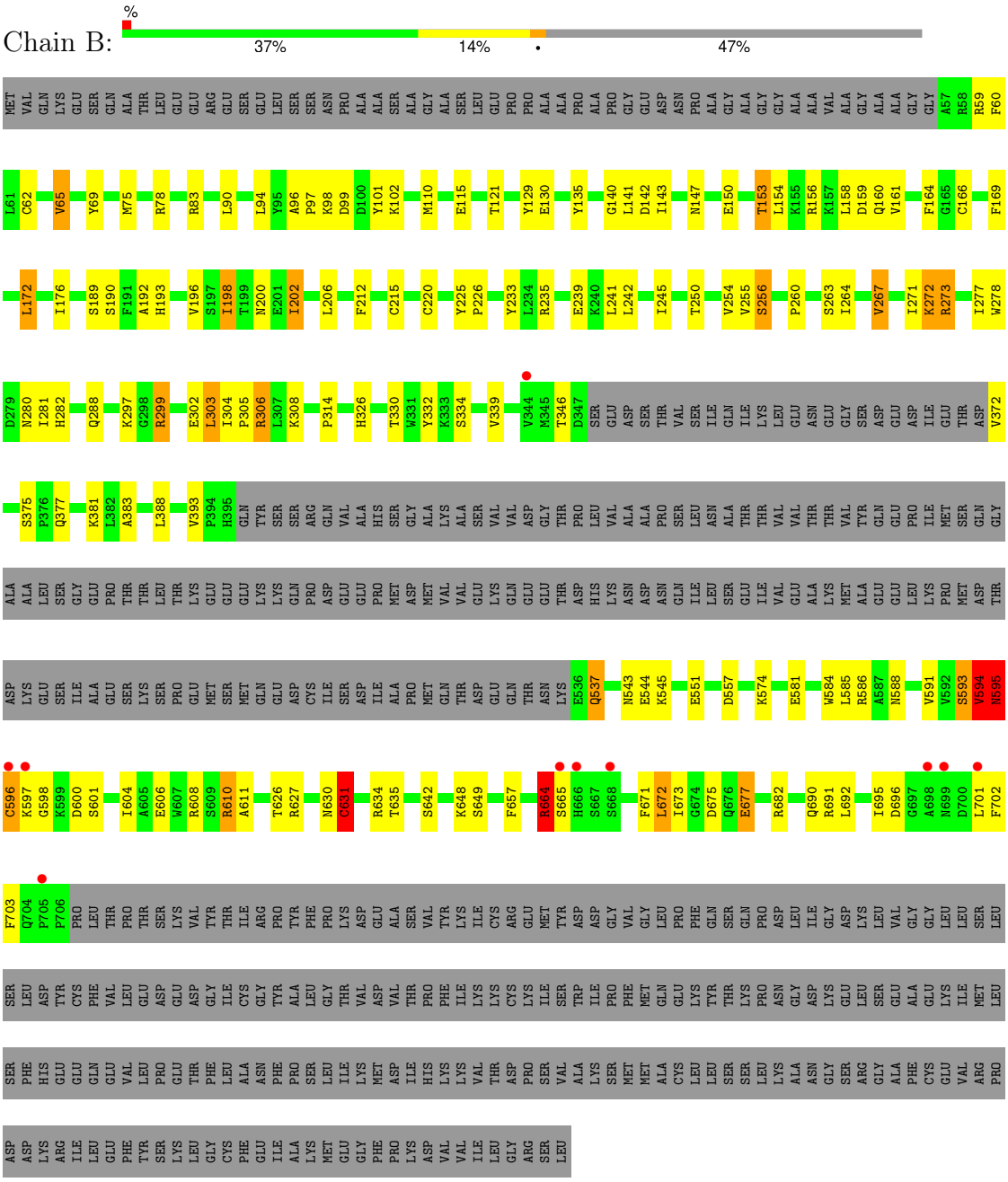
Chain A:





• Molecule 1: Protein O-GlcNAcase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	222.17Å 222.17Å 72.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	192.40 – 3.30 192.40 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (192.40-3.30) 100.0 (192.40-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.169 , 0.234 0.177 , 0.235	Depositor DCC
R_{free} test set	1483 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	77.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7880	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.58	0/4080	0.83	1/5536 (0.0%)
1	B	0.57	0/4021	0.81	1/5453 (0.0%)
All	All	0.58	0/8101	0.82	2/10989 (0.0%)

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	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	631	CYS	CB-CA-C	5.19	120.78	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	ARG	Sidechain
1	A	273	ARG	Sidechain
1	A	83[A]	ARG	Sidechain
1	A	83[B]	ARG	Sidechain
1	B	59	ARG	Sidechain
1	B	608	ARG	Sidechain
1	B	664	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	78	ARG	Sidechain

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	3965	0	3862	76	0
1	B	3914	0	3810	80	0
2	B	1	0	0	0	0
All	All	7880	0	7672	145	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 9.

All (145) 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:110:MET:HB3	1:B:160:GLN:HE22	1.49	0.77
1:A:300:SER:O	1:A:303:LEU:HD22	1.88	0.74
1:A:108:ARG:HH22	1:A:150:GLU:CD	1.92	0.73
1:B:585:LEU:HD21	1:B:611:ALA:HA	1.71	0.72
1:A:586:ARG:NH2	1:A:700:ASP:O	2.22	0.72
1:A:83[B]:ARG:HG2	1:A:129:TYR:CE1	2.25	0.72
1:B:190:SER:HB3	1:B:193:HIS:ND1	2.05	0.71
1:A:543:ASN:HD22	1:A:543:ASN:H	1.40	0.70
1:A:697:GLY:HA2	1:B:703:PHE:HD2	1.58	0.68
1:B:664:ARG:HB2	1:B:664:ARG:HH11	1.59	0.67
1:B:200:ASN:OD1	1:B:242:LEU:HD12	1.96	0.65
1:A:548:TYR:O	1:A:549:THR:HG23	1.97	0.65
1:B:537:GLN:HE21	1:B:537:GLN:HA	1.62	0.64
1:B:588:ASN:O	1:B:591:VAL:HG12	1.99	0.63
1:A:139:PRO:O	1:A:143:ILE:HB	1.98	0.63
1:A:650:ILE:HD11	1:B:288:GLN:CG	2.28	0.63
1:A:692:LEU:O	1:B:586:ARG:NH1	2.34	0.61
1:B:581:GLU:O	1:B:585:LEU:HD12	1.99	0.61
1:B:271:ILE:O	1:B:273:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:VAL:HG22	1:B:665:SER:HB2	1.84	0.60
1:A:193:HIS:CD2	1:A:236:THR:HG21	2.37	0.59
1:A:548:TYR:O	1:A:549:THR:CG2	2.50	0.58
1:B:537:GLN:HE21	1:B:537:GLN:CA	2.16	0.58
1:B:153:THR:HG23	1:B:156:ARG:NH2	2.19	0.58
1:A:561:LEU:CA	1:A:624:MET:HE1	2.35	0.57
1:A:375:SER:OG	1:A:377[A]:GLN:NE2	2.38	0.56
1:A:697:GLY:HA2	1:B:703:PHE:CD2	2.39	0.56
1:A:334:SER:O	1:A:335:ASN:HB2	2.05	0.56
1:A:302:GLU:O	1:A:305:PRO:HD2	2.05	0.56
1:B:302:GLU:OE1	1:B:306:ARG:NH1	2.39	0.56
1:A:108:ARG:NH2	1:A:150:GLU:OE2	2.40	0.55
1:A:634:ARG:HG3	1:A:634:ARG:HH11	1.70	0.55
1:A:300:SER:O	1:A:303:LEU:CD2	2.53	0.55
1:B:110:MET:HB3	1:B:160:GLN:NE2	2.22	0.55
1:A:124:SER:OG	1:A:127:ARG:NH2	2.40	0.54
1:A:304:ILE:N	1:A:305:PRO:CD	2.71	0.54
1:B:65:VAL:HB	1:B:94:LEU:HB3	1.90	0.54
1:A:561:LEU:N	1:A:624:MET:HE1	2.24	0.53
1:B:677:GLU:CG	1:B:677:GLU:O	2.57	0.53
1:A:227:ASN:HD21	1:A:230:GLN:HE21	1.56	0.53
1:A:96:ALA:N	1:A:97:PRO:CD	2.71	0.53
1:A:340:ARG:HD2	1:A:340:ARG:N	2.23	0.53
1:B:584:TRP:CZ2	1:B:610:ARG:NH2	2.77	0.53
1:A:271:ILE:O	1:A:273:ARG:HG2	2.10	0.52
1:B:242:LEU:O	1:B:273:ARG:NH2	2.42	0.51
1:A:159:ASP:OD2	1:A:205:TYR:OH	2.23	0.51
1:A:68:PHE:HB2	1:A:285:ASP:HB3	1.92	0.51
1:A:108:ARG:NH2	1:A:150:GLU:CD	2.64	0.51
1:B:585:LEU:HD21	1:B:611:ALA:CA	2.42	0.50
1:B:267:VAL:O	1:B:271:ILE:HG12	2.11	0.50
1:A:695:ILE:HD13	1:B:701:LEU:HD12	1.93	0.49
1:B:584:TRP:O	1:B:588:ASN:ND2	2.34	0.49
1:B:260:PRO:O	1:B:263:SER:HB3	2.11	0.49
1:A:544:GLU:OE2	1:B:147:ASN:HB2	2.12	0.49
1:B:154:LEU:HD23	1:B:202:ILE:HD11	1.94	0.49
1:B:584:TRP:CE2	1:B:610:ARG:NH2	2.78	0.49
1:B:62:CYS:SG	1:B:90:LEU:HD22	2.53	0.49
1:A:333:LYS:O	1:A:335:ASN:N	2.45	0.49
1:B:278:TRP:CD1	1:B:280:ASN:ND2	2.81	0.49
1:A:190:SER:HB3	1:A:193:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:HB	1:B:305:PRO:HD3	1.95	0.49
1:A:621:VAL:O	1:A:624:MET:HG3	2.13	0.48
1:A:677:GLU:OE1	1:A:704:GLN:NE2	2.45	0.48
1:A:631:CYS:O	1:B:101:TYR:OH	2.27	0.48
1:B:682:ARG:O	1:B:691:ARG:NH2	2.47	0.47
1:B:254:VAL:HG12	1:B:255:VAL:HG23	1.95	0.47
1:A:567:LEU:HB3	1:A:568:PRO:HD2	1.96	0.47
1:B:600:ASP:O	1:B:604:ILE:HG13	2.15	0.47
1:B:671:PHE:O	1:B:672:LEU:HD22	2.14	0.47
1:A:144:THR:HG21	1:B:544:GLU:HB3	1.95	0.46
1:A:601:SER:O	1:A:606:GLU:N	2.48	0.46
1:A:107:TRP:CZ2	1:A:143:ILE:HG13	2.50	0.46
1:A:250:THR:HA	1:A:278:TRP:O	2.16	0.46
1:B:129:TYR:O	1:B:130:GLU:HB2	2.15	0.46
1:B:595:ASN:HD22	1:B:596:CYS:N	2.13	0.46
1:B:326:HIS:CD2	1:B:383:ALA:HB2	2.51	0.46
1:A:204:GLN:NE2	1:A:242:LEU:HD11	2.30	0.45
1:B:584:TRP:CG	1:B:610:ARG:NH1	2.84	0.45
1:A:248:LEU:HD13	1:A:278:TRP:HE3	1.81	0.45
1:B:255:VAL:HG22	1:B:280:ASN:HB3	1.98	0.45
1:B:135:TYR:CG	1:B:161:VAL:HG11	2.51	0.45
1:B:664:ARG:HH11	1:B:664:ARG:CB	2.28	0.45
1:A:543:ASN:H	1:A:543:ASN:ND2	2.11	0.45
1:A:584:TRP:CE2	1:A:610:ARG:NH1	2.85	0.45
1:B:585:LEU:CD2	1:B:611:ALA:HA	2.46	0.45
1:A:218:GLU:HG2	1:A:223:PHE:O	2.16	0.45
1:A:629:SER:C	1:A:630:ASN:HD22	2.20	0.45
1:B:96:ALA:N	1:B:97:PRO:CD	2.80	0.45
1:A:557:ASP:CG	1:A:627:ARG:HH21	2.19	0.44
1:B:110:MET:CB	1:B:160:GLN:HE22	2.26	0.44
1:B:192:ALA:HB2	1:B:233:TYR:CD2	2.52	0.44
1:A:543:ASN:ND2	1:A:543:ASN:N	2.65	0.44
1:A:599:LYS:CB	1:A:604:ILE:HG13	2.47	0.44
1:B:69:TYR:CE1	1:B:98:LYS:HD2	2.52	0.44
1:B:198:ILE:O	1:B:202:ILE:HG13	2.17	0.44
1:B:235:ARG:O	1:B:239:GLU:HG3	2.18	0.44
1:B:60:PHE:CD2	1:B:332:TYR:CE1	3.05	0.44
1:A:634:ARG:HG3	1:A:634:ARG:NH1	2.30	0.44
1:A:636:ILE:H	1:A:636:ILE:HD12	1.82	0.43
1:B:172:LEU:HB3	1:B:215:CYS:HB3	1.99	0.43
1:B:281:ILE:HG23	1:B:282:HIS:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASN:OD1	1:B:242:LEU:CD1	2.65	0.43
1:B:102:LYS:HE3	1:B:115:GLU:OE1	2.19	0.43
1:B:225:TYR:HA	1:B:226:PRO:HA	1.80	0.43
1:B:630:ASN:O	1:B:631:CYS:C	2.57	0.43
1:A:582:PHE:HB2	1:A:614:PHE:CZ	2.53	0.43
1:B:200:ASN:CG	1:B:242:LEU:HD12	2.39	0.43
1:A:225:TYR:CD1	1:A:226:PRO:HA	2.54	0.42
1:A:304:ILE:N	1:A:305:PRO:HD3	2.34	0.42
1:A:543:ASN:HD22	1:A:543:ASN:N	2.05	0.42
1:B:606:GLU:O	1:B:610:ARG:HB2	2.20	0.42
1:A:77:GLN:NE2	1:A:318:PHE:CB	2.83	0.42
1:A:300:SER:HA	1:A:371:ASP:OD2	2.20	0.42
1:A:586:ARG:NH1	1:B:692:LEU:O	2.52	0.42
1:A:299:ARG:HD2	1:A:299:ARG:N	2.35	0.42
1:B:250:THR:O	1:B:256:SER:OG	2.38	0.42
1:A:703:PHE:HA	1:B:695:ILE:O	2.20	0.42
1:B:147:ASN:OD1	1:B:147:ASN:C	2.58	0.42
1:B:299:ARG:CD	1:B:299:ARG:N	2.83	0.42
1:B:220:CYS:HB3	1:B:250:THR:OG1	2.19	0.42
1:B:598:GLY:O	1:B:600:ASP:N	2.43	0.42
1:A:387:TRP:O	1:A:390:GLU:HB2	2.20	0.41
1:B:241:LEU:HD21	1:B:245:ILE:HG22	2.02	0.41
1:B:657:PHE:HA	1:B:671:PHE:CE1	2.55	0.41
1:B:303:LEU:HD12	1:B:303:LEU:HA	1.83	0.41
1:B:557:ASP:OD1	1:B:627:ARG:NH2	2.53	0.41
1:A:545:LYS:HD2	1:B:143:ILE:O	2.20	0.41
1:A:645:TRP:O	1:A:648:LYS:HG3	2.20	0.41
1:B:271:ILE:C	1:B:272:LYS:HG2	2.40	0.41
1:A:242:LEU:O	1:A:273:ARG:NH2	2.53	0.41
1:B:169:PHE:O	1:B:212:PHE:HA	2.20	0.41
1:A:563:ASP:OD2	1:A:573:PRO:HD2	2.20	0.41
1:A:634:ARG:HH11	1:A:634:ARG:CG	2.34	0.41
1:A:225:TYR:HA	1:A:226:PRO:HA	1.89	0.41
1:A:300:SER:C	1:A:302:GLU:N	2.74	0.41
1:A:537:GLN:HE21	1:A:537:GLN:HB2	1.69	0.41
1:A:674:GLY:O	1:A:675:ASP:OD1	2.39	0.41
1:A:682:ARG:O	1:A:687:GLY:HA3	2.21	0.41
1:B:160:GLN:HG2	1:B:164:PHE:CZ	2.56	0.41
1:A:107:TRP:CZ2	1:A:108:ARG:NH2	2.89	0.41
1:A:657:PHE:HA	1:A:671:PHE:CE1	2.56	0.41
1:B:196:VAL:HG12	1:B:200:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:SER:OG	1:B:377:GLN:NE2	2.54	0.40
1:A:707:PRO:O	1:A:709:THR:HG22	2.21	0.40
1:B:584:TRP:CD2	1:B:610:ARG:NH1	2.89	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	486/916 (53%)	425 (87%)	49 (10%)	12 (2%)	5 27
1	B	480/916 (52%)	431 (90%)	40 (8%)	9 (2%)	8 34
All	All	966/1832 (53%)	856 (89%)	89 (9%)	21 (2%)	6 30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	A	699	ASN
1	B	593	SER
1	B	597	LYS
1	A	334	SER
1	A	682	ARG
1	B	140	GLY
1	A	669	ALA
1	A	674	GLY
1	A	713	LYS
1	B	595	ASN
1	B	596	CYS
1	B	702	PHE
1	A	227	ASN
1	A	549	THR

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Mol	Chain	Res	Type
1	B	314	PRO
1	A	371	ASP
1	B	594	VAL
1	B	673	ILE
1	A	595	ASN
1	A	604	ILE

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	426/795 (54%)	378 (89%)	48 (11%)	6 22
1	B	418/795 (53%)	358 (86%)	60 (14%)	3 15
All	All	844/1590 (53%)	736 (87%)	108 (13%)	4 18

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	76	GLU
1	A	83[A]	ARG
1	A	83[B]	ARG
1	A	87	LYS
1	A	108	ARG
1	A	113	VAL
1	A	132	GLU
1	A	143	ILE
1	A	150	GLU
1	A	167	ARG
1	A	190	SER
1	A	201	GLU
1	A	229	SER
1	A	253	LYS
1	A	266	GLU
1	A	281	ILE

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Mol	Chain	Res	Type
1	A	299	ARG
1	A	301	THR
1	A	303	LEU
1	A	304	ILE
1	A	339	VAL
1	A	377[A]	GLN
1	A	377[B]	GLN
1	A	388	LEU
1	A	396	GLN
1	A	537	GLN
1	A	543	ASN
1	A	549	THR
1	A	554	THR
1	A	563	ASP
1	A	570	GLU
1	A	578	MET
1	A	583	GLN
1	A	594	VAL
1	A	600	ASP
1	A	622	MET
1	A	624	MET
1	A	630	ASN
1	A	634	ARG
1	A	648	LYS
1	A	651	MET
1	A	653	MET
1	A	654	VAL
1	A	675	ASP
1	A	676	GLN
1	A	691	ARG
1	A	714	VAL
1	B	65	VAL
1	B	75	MET
1	B	83	ARG
1	B	99	ASP
1	B	121	THR
1	B	141	LEU
1	B	142	ASP
1	B	150	GLU
1	B	153	THR
1	B	158	LEU
1	B	159	ASP

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Mol	Chain	Res	Type
1	B	166	CYS
1	B	172	LEU
1	B	176	ILE
1	B	189	SER
1	B	198	ILE
1	B	202	ILE
1	B	206	LEU
1	B	256	SER
1	B	264	ILE
1	B	267	VAL
1	B	272	LYS
1	B	273	ARG
1	B	277	ILE
1	B	297	LYS
1	B	299	ARG
1	B	303	LEU
1	B	306	ARG
1	B	308	LYS
1	B	330	THR
1	B	334	SER
1	B	339	VAL
1	B	346	THR
1	B	372	VAL
1	B	381	LYS
1	B	388	LEU
1	B	393	VAL
1	B	537	GLN
1	B	543	ASN
1	B	545	LYS
1	B	551	GLU
1	B	574	LYS
1	B	593	SER
1	B	594	VAL
1	B	595	ASN
1	B	601	SER
1	B	610	ARG
1	B	626	THR
1	B	631	CYS
1	B	634	ARG
1	B	635	THR
1	B	642	SER
1	B	648	LYS

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Mol	Chain	Res	Type
1	B	649	SER
1	B	664	ARG
1	B	672	LEU
1	B	675	ASP
1	B	677	GLU
1	B	690	GLN
1	B	696	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	103	HIS
1	A	163	GLN
1	A	193	HIS
1	A	204	GLN
1	A	230	GLN
1	A	288	GLN
1	A	326	HIS
1	A	395	HIS
1	A	537	GLN
1	A	543	ASN
1	A	583	GLN
1	A	630	ASN
1	A	670	GLN
1	B	230	GLN
1	B	280	ASN
1	B	326	HIS
1	B	335	ASN
1	B	377	GLN
1	B	537	GLN
1	B	543	ASN
1	B	595	ASN
1	B	630	ASN

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 monosaccharides 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, 95^{th} 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	490/916 (53%)	0.06	6 (1%)	79	78	46, 68, 125, 179	0
1	B	486/916 (53%)	0.09	10 (2%)	63	62	44, 72, 116, 175	0
All	All	976/1832 (53%)	0.08	16 (1%)	72	70	44, 70, 122, 179	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	602	ALA	6.1
1	B	666	HIS	4.9
1	B	699	ASN	4.0
1	A	601	SER	4.0
1	A	699	ASN	3.3
1	B	596	CYS	2.6
1	B	344	VAL	2.5
1	A	679	TRP	2.4
1	B	597	LYS	2.3
1	B	668	SER	2.2
1	B	665	SER	2.2
1	A	701	LEU	2.1
1	B	701	LEU	2.1
1	B	698	ALA	2.1
1	A	596	CYS	2.0
1	B	705	PRO	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 (i)

There are no monosaccharides 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.