



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:28 AM GMT

PDB ID : 2F4O
Title : The Mouse PNGase-HR23 Complex Reveals a Complete Remodulation of the Protein-Protein Interface Compared to its Yeast Orthologs
Authors : Zhao, G.; Zhou, X.; Wang, L.; Kisker, C.; Lennarz, W.J.; Schindelin, H.
Deposited on : 2005-11-23
Resolution : 2.26 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

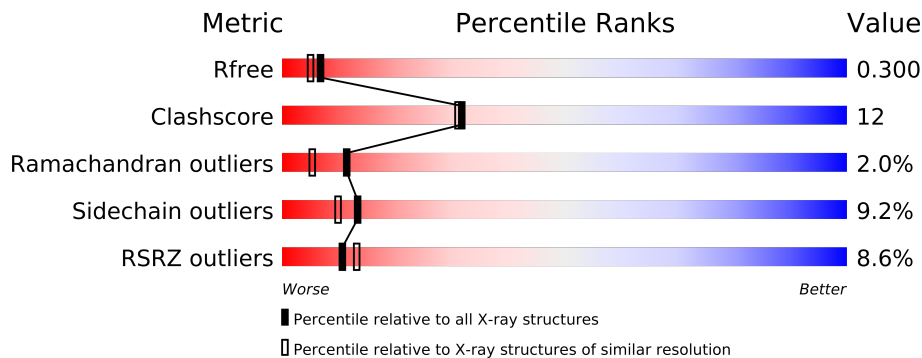
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.26 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. 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	A	295	
2	B	61	
3	I	5	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2966 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 peptide N-glycanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2409	1520	433	441	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	LEU	-	CLONING ARTIFACT	GB 30517852
A	452	GLU	-	CLONING ARTIFACT	GB 30517852
A	453	HIS	-	EXPRESSION TAG	GB 30517852
A	454	HIS	-	EXPRESSION TAG	GB 30517852
A	455	HIS	-	EXPRESSION TAG	GB 30517852
A	456	HIS	-	EXPRESSION TAG	GB 30517852
A	457	HIS	-	EXPRESSION TAG	GB 30517852
A	458	HIS	-	EXPRESSION TAG	GB 30517852

- Molecule 2 is a protein called XP-C repair complementing complex 58 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	61	Total	C	N	O	S	0	0	0
			505	318	95	90	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	333	GLY	-	CLONING ARTIFACT	UNP P54728

- Molecule 3 is a protein called PHQ-VAL-ALA-ASP-CF0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	0	0	1
			31	21	3	7			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Zn 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0

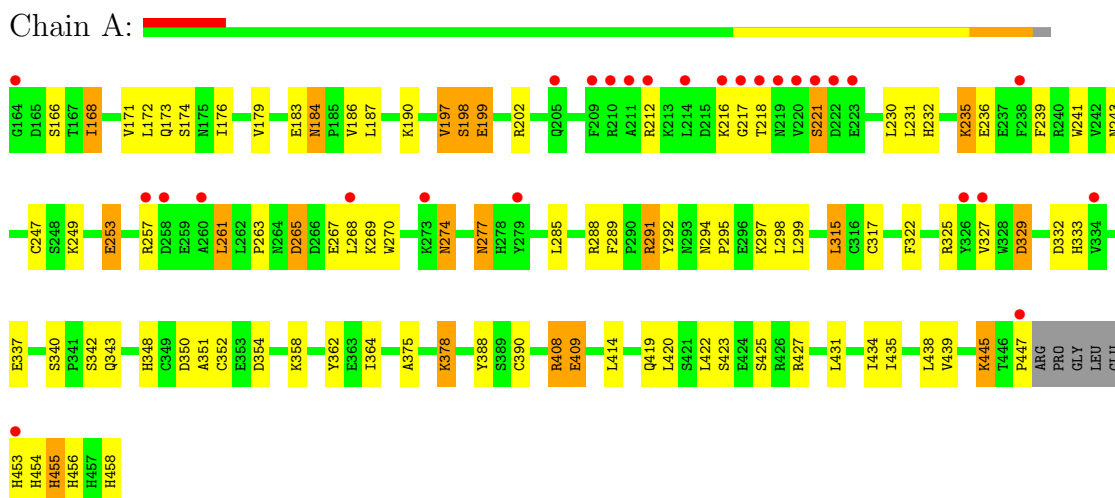
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total 17	O 17	0	0
6	B	1	Total 1	O 1	0	0

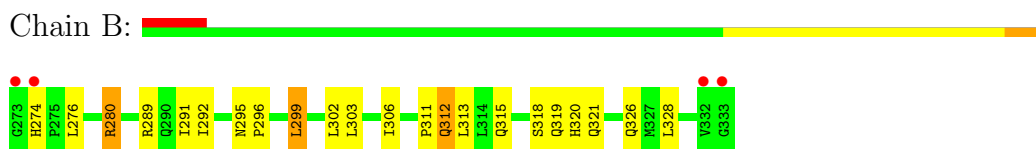
3 Residue-property plots

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: peptide N-glycanase



- Molecule 2: XP-C repair complementing complex 58 kDa protein



- Molecule 3: PHQ-VAL-ALA-ASP-CF0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.96Å 52.10Å 80.85Å 90.00° 113.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.26 35.40 – 2.26	Depositor EDS
% Data completeness (in resolution range)	83.2 (20.00-2.26) 83.2 (35.40-2.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.220 , 0.293 0.230 , 0.300	Depositor DCC
R_{free} test set	740 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 14571 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2966	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PHQ, ZN, CF0, CL

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	0.81	2/2465 (0.1%)	0.85	4/3329 (0.1%)
2	B	0.67	0/516	0.83	2/698 (0.3%)
3	I	0.91	0/19	2.05	1/25 (4.0%)
All	All	0.79	2/3000 (0.1%)	0.86	7/4052 (0.2%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	GLU	CD-OE2	8.15	1.34	1.25
1	A	425	SER	CB-OG	5.92	1.50	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ARG	NE-CZ-NH2	-7.63	116.48	120.30
2	B	280	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	291	ARG	NE-CZ-NH1	7.25	123.92	120.30
2	B	280	ARG	NE-CZ-NH2	-6.67	116.96	120.30
3	I	4	ASP	CB-CG-OD2	6.65	124.29	118.30
1	A	329	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	329	ASP	CB-CG-OD1	-5.20	113.62	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	455	HIS	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	A	2409	0	2355	57	0
2	B	505	0	501	12	0
3	I	31	0	24	1	0
4	A	2	0	0	0	0
5	A	1	0	0	1	0
6	A	17	0	0	1	0
6	B	1	0	0	0	0
All	All	2966	0	2880	67	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 12.

All (67) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:ILE:HD11	1:A:414:LEU:HD13	1.47	0.96
1:A:176:ILE:CD1	1:A:414:LEU:HD13	2.16	0.76
1:A:327:VAL:HG21	1:A:337:GLU:HG3	1.70	0.73
1:A:184:ASN:N	1:A:184:ASN:HD22	1.87	0.72
1:A:187:LEU:HG	1:A:315:LEU:HD11	1.74	0.69
1:A:294:ASN:HD22	1:A:295:PRO:HD2	1.57	0.68
1:A:419:GLN:HG2	1:A:422:LEU:HD12	1.76	0.66
1:A:295:PRO:HB2	1:A:315:LEU:HD12	1.78	0.63
1:A:232:HIS:O	1:A:236:GLU:HG2	1.98	0.63
1:A:390:CYS:SG	1:A:447:PRO:HB3	2.39	0.63
1:A:291:ARG:NH2	3:I:4:ASP:OD1	2.35	0.60
1:A:348:HIS:HD2	1:A:358:LYS:H	1.52	0.58
1:A:263:PRO:HG2	1:A:268:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:312:GLN:HA	2:B:315:GLN:HE21	1.69	0.57
1:A:176:ILE:HD13	1:A:414:LEU:HD22	1.90	0.53
2:B:319:GLN:HB2	2:B:320:HIS:CD2	2.44	0.52
1:A:184:ASN:ND2	1:A:184:ASN:N	2.57	0.52
1:A:348:HIS:HE1	1:A:362:TYR:OH	1.93	0.51
1:A:456:HIS:HE1	5:A:1:CL:CL	2.30	0.51
1:A:289:PHE:CE2	1:A:291:ARG:HD3	2.45	0.51
2:B:311:PRO:O	2:B:315:GLN:HG3	2.10	0.51
1:A:249:LYS:HB2	1:A:285:LEU:HD22	1.93	0.51
1:A:390:CYS:HB2	1:A:445:LYS:O	2.11	0.50
1:A:292:TYR:HB2	1:A:298:LEU:HD21	1.94	0.50
1:A:329:ASP:HB3	1:A:333:HIS:O	2.12	0.49
1:A:235:LYS:HG3	1:A:354:ASP:HB2	1.94	0.49
1:A:235:LYS:HB3	1:A:236:GLU:OE2	2.12	0.49
1:A:325:ARG:HD3	1:A:375:ALA:HB1	1.94	0.49
1:A:197:VAL:O	1:A:198:SER:C	2.50	0.49
1:A:420:LEU:HA	1:A:427:ARG:HH21	1.78	0.49
1:A:270:TRP:CE3	1:A:297:LYS:HB2	2.47	0.49
1:A:438:LEU:HD11	2:B:291:ILE:HD12	1.93	0.49
1:A:247:CYS:SG	1:A:285:LEU:HD23	2.53	0.48
1:A:431:LEU:HD13	2:B:295:ASN:ND2	2.29	0.48
1:A:172:LEU:O	1:A:176:ILE:HG13	2.13	0.48
1:A:350:ASP:OD2	1:A:362:TYR:OH	2.25	0.47
1:A:241:TRP:HZ3	1:A:352:CYS:SG	2.37	0.47
1:A:294:ASN:HD22	1:A:295:PRO:CD	2.26	0.47
2:B:289:ARG:HG2	2:B:328:LEU:HA	1.97	0.47
1:A:364:ILE:HG21	1:A:453:HIS:CB	2.45	0.47
1:A:267:GLU:OE1	1:A:288:ARG:NH1	2.48	0.47
1:A:265:ASP:O	1:A:269:LYS:HG2	2.16	0.46
1:A:231:LEU:CD2	1:A:351:ALA:HA	2.46	0.46
1:A:231:LEU:HD23	1:A:351:ALA:HA	1.98	0.45
1:A:455:HIS:ND1	1:A:458:HIS:HB2	2.32	0.45
2:B:306:ILE:HG23	2:B:313:LEU:HD23	1.99	0.44
1:A:197:VAL:O	1:A:199:GLU:N	2.51	0.44
1:A:434:ILE:HA	1:A:434:ILE:HD12	1.91	0.44
1:A:408:ARG:O	1:A:409:GLU:C	2.57	0.43
2:B:292:ILE:HD11	2:B:302:LEU:HD22	2.01	0.42
1:A:235:LYS:HE3	1:A:354:ASP:HB2	2.02	0.42
1:A:168:ILE:O	1:A:171:VAL:HG22	2.18	0.42
1:A:198:SER:O	1:A:202:ARG:HB2	2.20	0.42
1:A:337:GLU:OE2	1:A:388:TYR:OH	2.30	0.42
2:B:280:ARG:HH22	2:B:326:GLN:HE22	1.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:LEU:HD13	1:A:277:ASN:HB2	2.02	0.41
2:B:295:ASN:N	2:B:296:PRO:CD	2.84	0.41
1:A:332:ASP:HB2	6:A:12:HOH:O	2.20	0.41
1:A:435:ILE:O	1:A:439:VAL:HG23	2.21	0.41
2:B:318:SER:HA	2:B:321:GLN:HG3	2.02	0.41
2:B:299:LEU:HD22	2:B:303:LEU:HG	2.02	0.41
1:A:184:ASN:HB3	1:A:186:VAL:HG12	2.02	0.41
1:A:317:CYS:O	1:A:322:PHE:HB2	2.21	0.41
1:A:183:GLU:HG3	1:A:378:LYS:HB3	2.02	0.40
1:A:190:LYS:HG2	1:A:299:LEU:HD13	2.04	0.40
1:A:340:SER:OG	1:A:343:GLN:HG3	2.21	0.40
1:A:274:ASN:ND2	1:A:274:ASN:N	2.70	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	286/295 (97%)	258 (90%)	21 (7%)	7 (2%)	9	4
2	B	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
3	I	1/5 (20%)	1 (100%)	0	0	100	100
All	All	346/361 (96%)	316 (91%)	23 (7%)	7 (2%)	11	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	GLY
1	A	265	ASP
1	A	454	HIS
1	A	198	SER
1	A	221	SER
1	A	253	GLU
1	A	197	VAL

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	268/272 (98%)	242 (90%)	26 (10%)	12	8
2	B	57/57 (100%)	53 (93%)	4 (7%)	21	19
3	I	2/2 (100%)	2 (100%)	0	100	100
All	All	327/331 (99%)	297 (91%)	30 (9%)	13	10

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	168	ILE
1	A	173	GLN
1	A	174	SER
1	A	179	VAL
1	A	184	ASN
1	A	212	ARG
1	A	216	LYS
1	A	218	THR
1	A	221	SER
1	A	230	LEU
1	A	235	LYS
1	A	239	PHE
1	A	243	ASN
1	A	253	GLU
1	A	257	ARG
1	A	261	LEU
1	A	274	ASN
1	A	277	ASN
1	A	315	LEU
1	A	342	SER
1	A	378	LYS
1	A	408	ARG
1	A	409	GLU
1	A	423	SER
1	A	445	LYS
2	B	274	HIS

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Mol	Chain	Res	Type
2	B	276	LEU
2	B	299	LEU
2	B	312	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	184	ASN
1	A	274	ASN
1	A	277	ASN
1	A	294	ASN
1	A	348	HIS
1	A	456	HIS
2	B	287	GLN
2	B	295	ASN
2	B	304	GLN
2	B	305	GLN
2	B	315	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 ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	290/295 (98%)	0.53	27 (9%) 9 11	56, 64, 78, 87	0
2	B	61/61 (100%)	0.37	4 (6%) 18 21	60, 64, 73, 81	0
3	I	5/5 (100%)	-0.01	0 100 100	54, 55, 57, 104	0
All	All	356/361 (98%)	0.50	31 (8%) 11 13	54, 64, 78, 104	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	GLY	5.5
2	B	274	HIS	5.3
1	A	218	THR	4.9
1	A	220	VAL	4.7
1	A	209	PHE	4.4
1	A	453	HIS	4.3
2	B	273	GLY	4.0
1	A	221	SER	3.9
2	B	333	GLY	3.8
1	A	447	PRO	3.6
1	A	219	ASN	2.9
1	A	211	ALA	2.8
1	A	279	TYR	2.8
1	A	222	ASP	2.8
1	A	238	PHE	2.6
2	B	332	VAL	2.5
1	A	223	GLU	2.5
1	A	210	ARG	2.5
1	A	327	VAL	2.5
1	A	216	LYS	2.4
1	A	205	GLN	2.4
1	A	260	ALA	2.4
1	A	326	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	ASP	2.2
1	A	214	LEU	2.2
1	A	268	LEU	2.2
1	A	273	LYS	2.2
1	A	257	ARG	2.1
1	A	212	ARG	2.0
1	A	164	GLY	2.0
1	A	334	VAL	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CL	A	1	1/1	0.16	0.62	80,80,80,80	0
4	ZN	A	501	1/1	0.07	-1.64	68,68,68,68	0
4	ZN	A	502	1/1	0.04	-2.19	62,62,62,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.