Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2024 – 07:13 pm BST

PDB ID	:	8QH2
Title	:	Crystal structure of chimeric UAP1L1
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Deposited on	:	2023-09-06
Resolution	:	2.75 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:

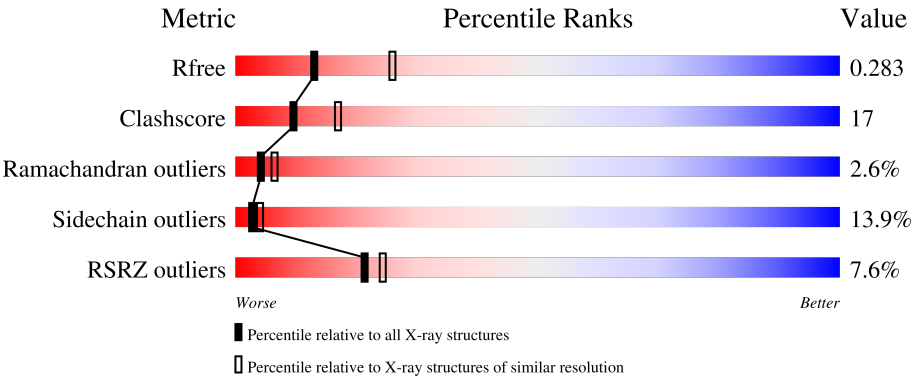
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	510	7% 52% 35% 7% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3810 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 UDP-N-acetylhexosamine pyrophosphorylase,UDP-N-acetylhexosamine pyrophosphorylase-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	3810	2437	664	693	16	89	0	0

There are 4 discrepancies between the modelled and reference sequences:

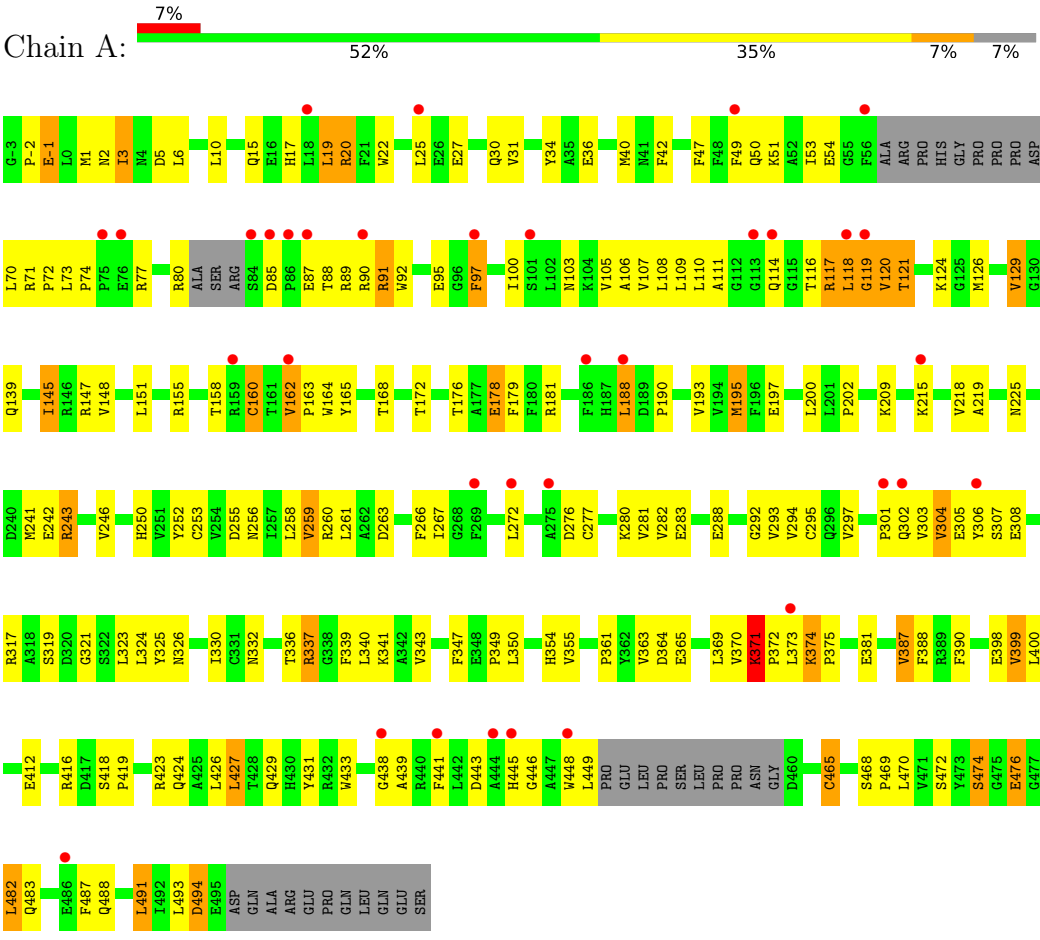
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q16222
A	-2	PRO	-	expression tag	UNP Q16222
A	-1	GLU	-	expression tag	UNP Q16222
A	0	LEU	-	expression tag	UNP Q16222

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: UDP-N-acetylhexosamine pyrophosphorylase,UDP-N-acetylhexosamine pyrophosphorylase-like protein 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	113.52Å 113.52Å 43.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 2.75 41.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.00-2.75) 100.0 (41.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158-000	Depositor
R, R_{free}	0.233 , 0.283 0.231 , 0.283	Depositor DCC
R_{free} test set	672 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 79.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3810	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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	0.47	0/3898	0.66	0/5274

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	3810	0	3772	128	0
All	All	3810	0	3772	128	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 (128) 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:19:LEU:HD12	1:A:22:TRP:HB2	1.59	0.84
1:A:256:ASN:HB3	1:A:259:VAL:HG22	1.63	0.80
1:A:100:ILE:HG13	1:A:105:VAL:HG21	1.69	0.74
1:A:172:THR:O	1:A:176:THR:HG22	1.88	0.72
1:A:238:LEU:HA	1:A:241:MET:HE2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TRP:O	1:A:30:GLN:NE2	2.23	0.71
1:A:250:HIS:NE2	1:A:332:ASN:OD1	2.21	0.70
1:A:110:LEU:HD13	1:A:225:ASN:HB2	1.75	0.69
1:A:304:VAL:HG23	1:A:308:GLU:HB2	1.75	0.69
1:A:323:LEU:O	1:A:326:ASN:ND2	2.27	0.67
1:A:336:THR:HG23	1:A:339:PHE:H	1.59	0.67
1:A:72:PRO:HG3	1:A:324:LEU:HD11	1.75	0.66
1:A:474:SER:N	1:A:476:GLU:OE2	2.25	0.66
1:A:73:LEU:HG	1:A:295:CYS:HA	1.76	0.66
1:A:443:ASP:N	1:A:446:GLY:O	2.20	0.66
1:A:363:VAL:HG23	1:A:369:LEU:HG	1.79	0.65
1:A:116:THR:O	1:A:118:LEU:N	2.30	0.65
1:A:258:LEU:HD23	1:A:426:LEU:HD12	1.77	0.64
1:A:343:VAL:HA	1:A:347:PHE:HD2	1.62	0.63
1:A:439:ALA:HB2	1:A:482:LEU:HB3	1.82	0.61
1:A:178:GLU:HA	1:A:181:ARG:HD2	1.82	0.61
1:A:17:HIS:CE1	1:A:209:LYS:HB3	2.36	0.61
1:A:1:MET:HE1	1:A:31:VAL:HG13	1.83	0.60
1:A:47:PHE:CZ	1:A:51:LYS:HE2	2.36	0.60
1:A:246:VAL:O	1:A:337:ARG:NH1	2.34	0.60
1:A:119:GLY:O	1:A:121:THR:N	2.35	0.60
1:A:423:ARG:HG2	1:A:427:LEU:HD23	1.82	0.60
1:A:294:VAL:HG22	1:A:303:VAL:HG22	1.85	0.59
1:A:145:ILE:HD12	1:A:162:VAL:HG13	1.84	0.58
1:A:242:GLU:HG3	1:A:337:ARG:NH2	2.19	0.58
1:A:10:LEU:HD22	1:A:15:GLN:HB2	1.86	0.57
1:A:70:LEU:HG	1:A:297:VAL:HG22	1.88	0.56
1:A:263:ASP:O	1:A:267:ILE:HD12	2.05	0.56
1:A:190:PRO:HA	1:A:193:VAL:HG12	1.86	0.56
1:A:106:ALA:HA	1:A:162:VAL:HG23	1.88	0.55
1:A:20:ARG:HE	1:A:20:ARG:HA	1.71	0.55
1:A:253:CYS:HB3	1:A:255:ASP:OD1	2.07	0.55
1:A:317:ARG:NH1	1:A:321:GLY:O	2.39	0.55
1:A:27:GLU:O	1:A:31:VAL:HG23	2.07	0.55
1:A:145:ILE:HA	1:A:148:VAL:HG12	1.90	0.54
1:A:108:LEU:HA	1:A:165:TYR:O	2.08	0.53
1:A:343:VAL:HA	1:A:347:PHE:CD2	2.43	0.53
1:A:339:PHE:O	1:A:343:VAL:HG13	2.09	0.52
1:A:118:LEU:HG	1:A:124:LYS:HD3	1.90	0.52
1:A:1:MET:HB2	1:A:34:TYR:CE2	2.45	0.51
1:A:25:LEU:HD11	1:A:215:LYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:MET:HE1	1:A:202:PRO:HG3	1.92	0.51
1:A:90:ARG:HG2	1:A:91:ARG:HH21	1.75	0.51
1:A:239:GLU:O	1:A:243:ARG:N	2.43	0.51
1:A:280:LYS:HB2	1:A:332:ASN:HB3	1.91	0.51
1:A:494:ASP:N	1:A:494:ASP:OD1	2.43	0.50
1:A:147:ARG:HD3	1:A:470:LEU:O	2.11	0.50
1:A:337:ARG:HD2	1:A:341:LYS:HE2	1.93	0.50
1:A:349:PRO:HB2	1:A:350:LEU:HD12	1.94	0.50
1:A:292:GLY:HA2	1:A:305:GLU:HA	1.94	0.50
1:A:108:LEU:HG	1:A:165:TYR:HB2	1.94	0.49
1:A:288:GLU:OE1	1:A:288:GLU:N	2.41	0.49
1:A:361:PRO:HA	1:A:371:LYS:HA	1.94	0.49
1:A:129:VAL:HG12	1:A:131:LEU:HD13	1.94	0.49
1:A:145:ILE:HD11	1:A:188:LEU:HD21	1.94	0.49
1:A:242:GLU:HA	1:A:337:ARG:CZ	2.42	0.49
1:A:282:VAL:HG12	1:A:399:VAL:O	2.12	0.49
1:A:95:GLU:OE2	1:A:272:LEU:HB2	2.13	0.49
1:A:2:ASN:ND2	1:A:5:ASP:HB2	2.28	0.48
1:A:111:ALA:O	1:A:168:THR:HA	2.13	0.48
1:A:429:GLN:OE1	1:A:433:TRP:NE1	2.45	0.48
1:A:20:ARG:HA	1:A:20:ARG:NE	2.29	0.48
1:A:25:LEU:HD21	1:A:215:LYS:HB2	1.95	0.48
1:A:293:VAL:HG11	1:A:325:TYR:HB3	1.97	0.47
1:A:482:LEU:HD12	1:A:487:PHE:CZ	2.49	0.47
1:A:17:HIS:HE1	1:A:209:LYS:HB3	1.79	0.47
1:A:118:LEU:O	1:A:120:VAL:N	2.48	0.47
1:A:232:LEU:HD13	1:A:238:LEU:HD11	1.97	0.47
1:A:305:GLU:O	1:A:308:GLU:N	2.39	0.47
1:A:109:LEU:HD21	1:A:138:TYR:HE1	1.79	0.47
1:A:92:TRP:N	1:A:92:TRP:CD1	2.80	0.46
1:A:106:ALA:HA	1:A:163:PRO:HD2	1.97	0.46
1:A:129:VAL:HG22	1:A:419:PRO:HA	1.98	0.46
1:A:364:ASP:OD1	1:A:365:GLU:N	2.44	0.46
1:A:40:MET:HE2	1:A:42:PHE:CE1	2.51	0.46
1:A:91:ARG:O	1:A:95:GLU:HG2	2.15	0.46
1:A:276:ASP:OD1	1:A:276:ASP:N	2.44	0.46
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.66	0.45
1:A:374:LYS:HD2	1:A:375:PRO:O	2.15	0.45
1:A:252:TYR:CZ	1:A:261:LEU:HD21	2.51	0.45
1:A:126:MET:HG2	1:A:179:PHE:CD2	2.52	0.45
1:A:478:LEU:HB3	1:A:482:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:C	1:A:87:GLU:H	2.19	0.45
1:A:85:ASP:OD2	1:A:88:THR:OG1	2.23	0.45
1:A:347:PHE:HB3	1:A:390:PHE:CE2	2.53	0.44
1:A:323:LEU:HA	1:A:323:LEU:HD23	1.64	0.43
1:A:49:PHE:CE2	1:A:53:ILE:HD11	2.53	0.43
1:A:19:LEU:HD13	1:A:19:LEU:HA	1.72	0.43
1:A:107:VAL:HG23	1:A:164:TRP:HA	2.01	0.43
1:A:465:CYS:HB2	1:A:491:LEU:HD23	2.00	0.43
1:A:50:GLN:O	1:A:54:GLU:HG3	2.18	0.43
1:A:151:LEU:O	1:A:155:ARG:HB2	2.19	0.43
1:A:232:LEU:HB3	1:A:238:LEU:HD13	2.01	0.43
1:A:70:LEU:O	1:A:71:ARG:HD2	2.19	0.43
1:A:20:ARG:HE	1:A:20:ARG:CA	2.32	0.43
1:A:168:THR:O	1:A:197:GLU:HA	2.18	0.43
1:A:312:GLU:N	1:A:312:GLU:OE1	2.52	0.43
1:A:103:ASN:OD1	1:A:160:CYS:HB2	2.20	0.42
1:A:276:ASP:O	1:A:336:THR:HG22	2.19	0.42
1:A:77:ARG:CD	1:A:301:PRO:HG3	2.49	0.42
1:A:263:ASP:O	1:A:266:PHE:N	2.53	0.42
1:A:339:PHE:HE2	1:A:387:VAL:HG13	1.83	0.42
1:A:90:ARG:NE	1:A:90:ARG:HA	2.34	0.42
1:A:97:PHE:CZ	1:A:151:LEU:HB3	2.55	0.42
1:A:354:HIS:N	1:A:381:GLU:O	2.33	0.42
1:A:40:MET:CE	1:A:202:PRO:HG3	2.50	0.41
1:A:371:LYS:H	1:A:371:LYS:HG2	1.62	0.41
1:A:85:ASP:O	1:A:87:GLU:N	2.53	0.41
1:A:176:THR:HG23	1:A:195:MET:HE1	2.02	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.58	0.41
1:A:469:PRO:HA	1:A:472:SER:O	2.20	0.41
1:A:260:ARG:HB3	1:A:263:ASP:HB2	2.02	0.41
1:A:431:TYR:HE1	1:A:441:PHE:CD1	2.37	0.41
1:A:302:GLN:HB2	1:A:388:PHE:HB2	2.02	0.41
1:A:36:GLU:OE2	1:A:218:VAL:HB	2.20	0.41
1:A:117:ARG:NE	1:A:412:GLU:OE1	2.43	0.41
1:A:330:ILE:HB	1:A:405:PHE:CD1	2.56	0.41
1:A:480:VAL:H	1:A:480:VAL:HG12	1.62	0.41
1:A:281:VAL:CG2	1:A:398:GLU:HG2	2.51	0.40
1:A:343:VAL:HA	1:A:347:PHE:HB2	2.03	0.40
1:A:438:GLY:HA3	1:A:483:GLN:HA	2.03	0.40
1:A:97:PHE:HA	1:A:100:ILE:HD13	2.02	0.40
1:A:3:ILE:HD13	1:A:6:LEU:HB3	2.02	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	468/510 (92%)	406 (87%)	50 (11%)	12 (3%)	4 6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	PRO
1	A	372	PRO
1	A	117	ARG
1	A	119	GLY
1	A	120	VAL
1	A	306	TYR
1	A	219	ALA
1	A	-1	GLU
1	A	74	PRO
1	A	448	TRP
1	A	371	LYS
1	A	374	LYS

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	403/432 (93%)	347 (86%)	56 (14%)	3 4

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	GLU
1	A	3	ILE
1	A	19	LEU
1	A	20	ARG
1	A	69	ARG
1	A	80	ARG
1	A	89	ARG
1	A	91	ARG
1	A	97	PHE
1	A	114	GLN
1	A	118	LEU
1	A	121	THR
1	A	129	VAL
1	A	131	LEU
1	A	137	LEU
1	A	139	GLN
1	A	145	ILE
1	A	158	THR
1	A	160	CYS
1	A	162	VAL
1	A	178	GLU
1	A	188	LEU
1	A	195	MET
1	A	200	LEU
1	A	243	ARG
1	A	259	VAL
1	A	277	CYS
1	A	283	GLU
1	A	304	VAL
1	A	307	SER
1	A	319	SER
1	A	337	ARG
1	A	355	VAL
1	A	370	VAL
1	A	371	LYS
1	A	373	LEU
1	A	387	VAL
1	A	399	VAL
1	A	400	LEU
1	A	403	GLU
1	A	416	ARG
1	A	418	SER

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Mol	Chain	Res	Type
1	A	424	GLN
1	A	427	LEU
1	A	445	HIS
1	A	449	LEU
1	A	465	CYS
1	A	468	SER
1	A	474	SER
1	A	476	GLU
1	A	480	VAL
1	A	482	LEU
1	A	488	GLN
1	A	491	LEU
1	A	493	LEU
1	A	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	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

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	476/510 (93%)	0.75	36 (7%) 21 24	48, 79, 122, 165	76 (15%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	HIS	6.5
1	A	87	GLU	5.8
1	A	119	GLY	4.3
1	A	186	PHE	3.9
1	A	118	LEU	3.0
1	A	438	GLY	3.0
1	A	272	LEU	2.8
1	A	162	VAL	2.8
1	A	84	SER	2.7
1	A	275	ALA	2.7
1	A	373	LEU	2.7
1	A	86	PRO	2.7
1	A	444	ALA	2.7
1	A	486	GLU	2.6
1	A	302	GLN	2.5
1	A	49	PHE	2.5
1	A	314	ALA	2.4
1	A	306	TYR	2.4
1	A	114	GLN	2.3
1	A	97	PHE	2.3
1	A	441	PHE	2.3
1	A	85	ASP	2.3
1	A	301	PRO	2.2
1	A	188	LEU	2.2
1	A	56	PHE	2.2
1	A	269	PHE	2.2
1	A	25	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	75	PRO	2.1
1	A	76	GLU	2.1
1	A	448	TRP	2.1
1	A	113	GLY	2.1
1	A	90	ARG	2.1
1	A	159	ARG	2.1
1	A	215	LYS	2.0
1	A	18	LEU	2.0
1	A	101	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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.