



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:35 PM UTC

PDB ID : 5H0I / pdb_00005h0i
Title : Structure of OaAEP1 asparaginyl peptide ligase in its proenzyme form
Authors : Yang, R.; Wong, Y.H.; Lescar, J.; Wu, B.
Deposited on : 2016-10-04
Resolution : 2.56 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

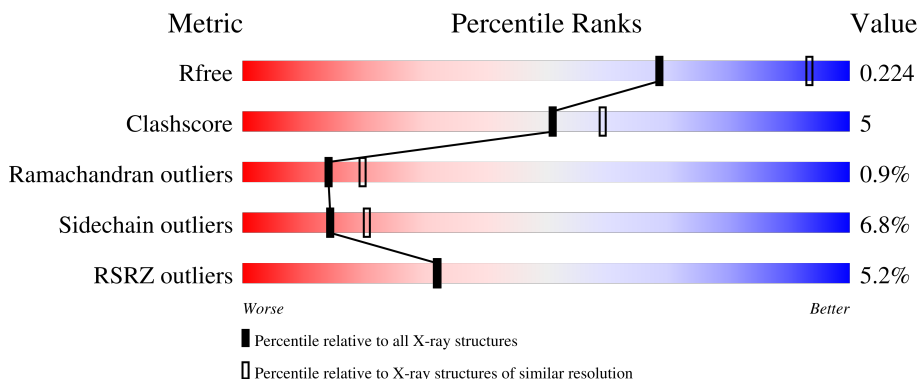
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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 $\leq 5\%$. 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	448	4% 73% 13% • 11%
1	B	448	5% 72% 15% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6494 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 Asparaginyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3101	1954	531	599	17			
1	B	400	Total	C	N	O	S	0	0	0
			3101	1956	530	598	17			

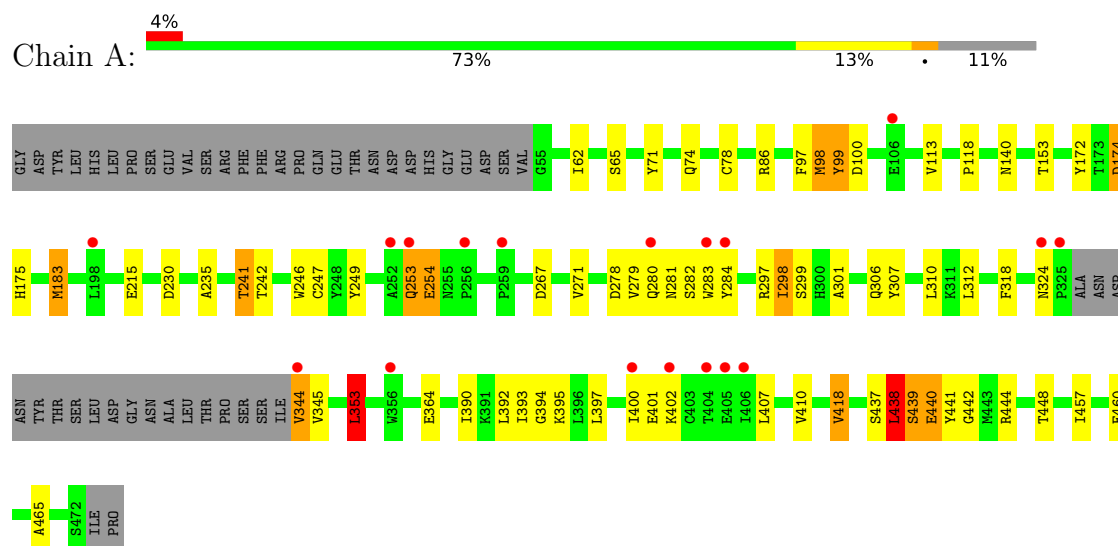
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	138	Total	O	0	0
			138	138		
2	B	154	Total	O	0	0
			154	154		

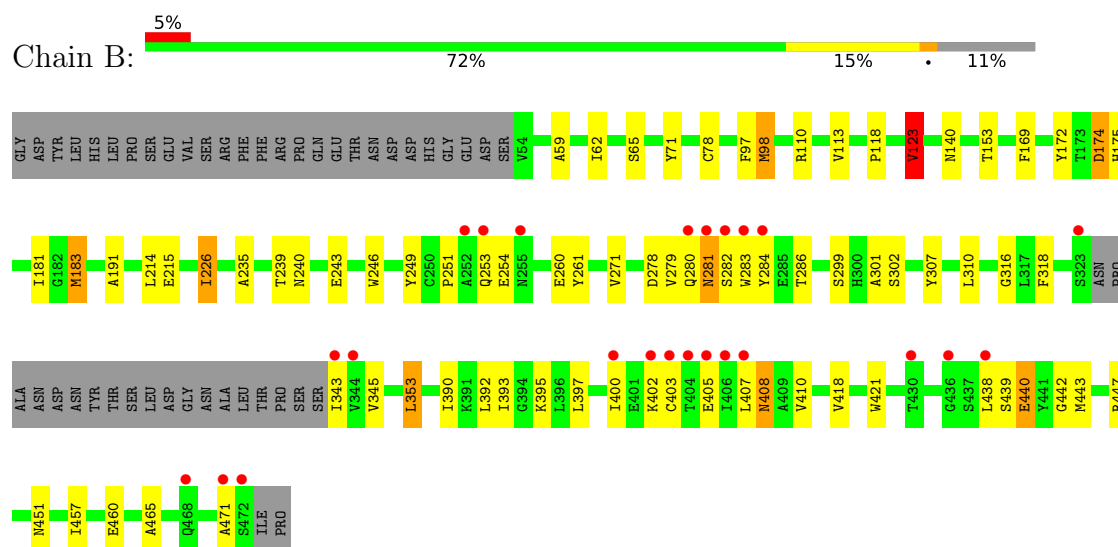
3 Residue-property plots [i](#)

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: Asparaginyl endopeptidase



- Molecule 1: Asparaginyl endopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.73Å 70.21Å 118.28Å 90.00° 117.14° 90.00°	Depositor
Resolution (Å)	71.72 – 2.56 71.72 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.6 (71.72-2.56) 99.6 (71.72-2.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.186 , 0.224 0.194 , 0.224	Depositor DCC
R_{free} test set	530 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6494	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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, 0.333 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	0.88	1/3176 (0.0%)	1.42	23/4309 (0.5%)
1	B	0.88	2/3175 (0.1%)	1.40	22/4307 (0.5%)
All	All	0.88	3/6351 (0.0%)	1.41	45/8616 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	MET	SD-CE	-7.04	1.61	1.79
1	A	183	MET	SD-CE	-5.86	1.65	1.79
1	B	240	ASN	CA-CB	5.00	1.59	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	VAL	CB-CA-C	7.96	119.21	110.62
1	B	471	ALA	N-CA-C	-7.32	104.35	113.28
1	B	239	THR	CA-C-N	6.73	132.37	121.74
1	B	239	THR	C-N-CA	6.73	132.37	121.74
1	B	71	TYR	CA-C-N	6.37	128.81	120.28
1	B	71	TYR	C-N-CA	6.37	128.81	120.28
1	A	283	TRP	CA-C-N	6.36	129.44	120.28
1	A	283	TRP	C-N-CA	6.36	129.44	120.28
1	A	99	TYR	CA-C-N	-6.22	110.76	122.27
1	A	99	TYR	C-N-CA	-6.22	110.76	122.27
1	A	100	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	71	TYR	CA-C-N	6.05	128.67	120.38
1	A	71	TYR	C-N-CA	6.05	128.67	120.38
1	B	123	VAL	N-CA-CB	-6.05	105.13	112.33
1	B	283	TRP	CA-C-N	6.03	128.96	120.28
1	B	283	TRP	C-N-CA	6.03	128.96	120.28
1	B	280	GLN	CA-C-N	5.99	129.62	121.05
1	B	280	GLN	C-N-CA	5.99	129.62	121.05
1	A	99	TYR	N-CA-C	-5.98	101.05	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	ASN	N-CA-C	-5.76	105.44	112.88
1	A	280	GLN	CA-C-N	5.72	129.23	121.05
1	A	280	GLN	C-N-CA	5.72	129.23	121.05
1	B	471	ALA	CA-C-N	5.71	131.98	121.70
1	B	471	ALA	C-N-CA	5.71	131.98	121.70
1	B	407	LEU	N-CA-C	-5.59	104.69	113.02
1	A	390	ILE	N-CA-CB	5.58	117.72	110.57
1	A	298	ILE	N-CA-CB	-5.58	106.07	112.21
1	B	278	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	418	VAL	N-CA-CB	-5.46	104.21	112.35
1	A	278	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	390	ILE	N-CA-CB	5.40	117.48	110.57
1	A	97	PHE	CA-CB-CG	5.38	119.18	113.80
1	B	451	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	438	LEU	N-CA-C	-5.26	105.09	112.25
1	A	298	ILE	CA-C-N	5.26	128.70	120.82
1	A	298	ILE	C-N-CA	5.26	128.70	120.82
1	A	395	LYS	CA-C-N	5.24	127.82	120.28
1	A	395	LYS	C-N-CA	5.24	127.82	120.28
1	B	281	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	97	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	353	LEU	CA-C-N	5.08	127.04	120.44
1	A	353	LEU	C-N-CA	5.08	127.04	120.44
1	B	395	LYS	CA-C-N	5.08	127.59	120.28
1	B	395	LYS	C-N-CA	5.08	127.59	120.28
1	A	230	ASP	CA-CB-CG	5.06	117.66	112.60

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	3101	0	2970	31	0
1	B	3101	0	2977	32	0
2	A	138	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	154	0	0	0	0
All	All	6494	0	5947	63	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 5.

All (63) 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:174:ASP:CG	1:B:175:HIS:H	1.53	1.16
1:A:174:ASP:CG	1:A:175:HIS:H	1.49	1.12
1:B:174:ASP:CG	1:B:175:HIS:N	2.30	0.88
1:A:174:ASP:CG	1:A:175:HIS:N	2.26	0.81
1:A:394:GLY:HA3	1:A:407:LEU:HD11	1.70	0.73
1:B:140:ASN:HD21	1:B:153:THR:H	1.37	0.73
1:A:140:ASN:HD21	1:A:153:THR:H	1.38	0.70
1:A:246:TRP:CD1	1:A:301:ALA:HB1	2.29	0.68
1:B:246:TRP:CD1	1:B:301:ALA:HB1	2.30	0.67
1:B:78:CYS:HB2	1:B:123:VAL:HG13	1.79	0.65
1:B:251:PRO:HD2	1:B:353:LEU:HD21	1.79	0.64
1:A:62:ILE:HD11	1:A:183:MET:HE1	1.81	0.62
1:A:438:LEU:HA	1:A:442:GLY:HA3	1.82	0.61
1:B:78:CYS:SG	1:B:98:MET:HE1	2.41	0.61
1:A:345:VAL:HG21	1:A:353:LEU:HD13	1.83	0.60
1:A:78:CYS:SG	1:A:98:MET:HE1	2.44	0.58
1:A:241:THR:HG22	1:A:242:THR:HG23	1.86	0.57
1:B:62:ILE:HD11	1:B:183:MET:HE1	1.85	0.57
1:A:65:SER:HB3	1:A:174:ASP:OD1	2.06	0.55
1:A:441:TYR:O	1:A:444:ARG:HG2	2.07	0.55
1:B:78:CYS:CB	1:B:123:VAL:HG13	2.38	0.53
1:B:281:ASN:HB3	1:B:284:TYR:HB2	1.89	0.53
1:A:306:GLN:HB3	1:A:310:LEU:HD22	1.91	0.53
1:A:281:ASN:HB3	1:A:284:TYR:HB2	1.90	0.53
1:B:397:LEU:HD13	1:B:465:ALA:HB2	1.91	0.52
1:A:407:LEU:HB3	1:A:448:THR:HG23	1.92	0.52
1:A:183:MET:HE3	1:A:183:MET:HA	1.91	0.51
1:B:183:MET:HE3	1:B:183:MET:HA	1.92	0.51
1:B:191:ALA:HB1	1:B:226:ILE:HD13	1.93	0.51
1:A:393:ILE:O	1:A:397:LEU:HB2	2.11	0.51
1:A:397:LEU:HD13	1:A:465:ALA:HB2	1.92	0.51
1:A:281:ASN:HB3	1:A:284:TYR:CB	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD21	1:A:457:ILE:HG21	1.94	0.50
1:B:281:ASN:HB3	1:B:284:TYR:CB	2.42	0.50
1:B:393:ILE:O	1:B:397:LEU:HB2	2.12	0.49
1:A:74:GLN:OE1	1:A:99:TYR:O	2.31	0.49
1:A:253:GLN:HG3	1:A:344:VAL:HA	1.94	0.49
1:B:397:LEU:HD21	1:B:457:ILE:HG21	1.95	0.49
1:B:447:ARG:HH11	1:B:447:ARG:HG2	1.80	0.47
1:A:439:SER:O	1:A:440:GLU:HB2	2.16	0.45
1:A:235:ALA:HB3	1:A:307:TYR:HB2	1.99	0.45
1:B:235:ALA:HB3	1:B:307:TYR:HB2	2.00	0.44
1:A:247:CYS:HA	1:A:267:ASP:HA	2.00	0.44
1:B:175:HIS:HB2	1:B:443:MET:HE1	2.01	0.43
1:A:86:ARG:HH11	1:A:324:ASN:ND2	2.17	0.43
1:B:438:LEU:HA	1:B:442:GLY:HA3	2.00	0.43
1:B:439:SER:O	1:B:440:GLU:C	2.61	0.43
1:B:243:GLU:OE1	1:B:302:SER:HA	2.19	0.42
1:B:282:SER:HB3	1:B:318:PHE:HB3	2.00	0.42
1:B:65:SER:HB3	1:B:174:ASP:OD1	2.19	0.42
1:B:118:PRO:HD3	1:B:249:TYR:CG	2.54	0.42
1:A:118:PRO:HD3	1:A:249:TYR:CD1	2.55	0.42
1:A:253:GLN:HG2	1:A:254:GLU:H	1.85	0.42
1:A:438:LEU:HD12	1:A:442:GLY:HA3	2.01	0.42
1:A:282:SER:HB3	1:A:318:PHE:HB3	2.00	0.41
1:B:191:ALA:HB3	1:B:421:TRP:CH2	2.55	0.41
1:B:286:THR:HA	1:B:316:GLY:HA2	2.01	0.41
1:B:110:ARG:HD3	1:B:261:TYR:OH	2.21	0.41
1:B:172:TYR:CD1	1:B:172:TYR:C	2.99	0.41
1:A:172:TYR:CD1	1:A:172:TYR:C	2.99	0.41
1:B:345:VAL:HG21	1:B:353:LEU:HD13	2.03	0.40
1:B:59:ALA:HA	1:B:169:PHE:O	2.21	0.40
1:B:181:ILE:HG21	1:B:214:LEU:HD21	2.03	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	396/448 (88%)	375 (95%)	17 (4%)	4 (1%)	12	17
1	B	396/448 (88%)	376 (95%)	17 (4%)	3 (1%)	16	22
All	All	792/896 (88%)	751 (95%)	34 (4%)	7 (1%)	14	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ASP
1	A	254	GLU
1	A	401	GLU
1	B	174	ASP
1	A	440	GLU
1	B	254	GLU
1	B	440	GLU

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	329/372 (88%)	306 (93%)	23 (7%)	14	19
1	B	329/372 (88%)	307 (93%)	22 (7%)	15	21
All	All	658/744 (88%)	613 (93%)	45 (7%)	14	20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	MET
1	A	113	VAL
1	A	215	GLU
1	A	241	THR
1	A	253	GLN
1	A	271	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	279	VAL
1	A	297	ARG
1	A	298	ILE
1	A	299	SER
1	A	312	LEU
1	A	344	VAL
1	A	353	LEU
1	A	364	GLU
1	A	392	LEU
1	A	400	ILE
1	A	402	LYS
1	A	410	VAL
1	A	418	VAL
1	A	437	SER
1	A	438	LEU
1	A	439	SER
1	A	460	GLU
1	B	98	MET
1	B	113	VAL
1	B	123	VAL
1	B	215	GLU
1	B	226	ILE
1	B	253	GLN
1	B	260	GLU
1	B	271	VAL
1	B	279	VAL
1	B	299	SER
1	B	310	LEU
1	B	343	ILE
1	B	353	LEU
1	B	392	LEU
1	B	400	ILE
1	B	402	LYS
1	B	403	CYS
1	B	405	GLU
1	B	408	ASN
1	B	410	VAL
1	B	418	VAL
1	B	460	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	195	ASN
1	A	202	HIS
1	A	290	GLN
1	A	293	HIS
1	A	306	GLN
1	A	324	ASN
1	A	354	HIS
1	A	461	GLN
1	B	140	ASN
1	B	195	ASN
1	B	293	HIS
1	B	306	GLN
1	B	385	HIS
1	B	408	ASN
1	B	451	ASN
1	B	461	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 ⓘ

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	400/448 (89%)	0.43	18 (4%) 38 39	34, 70, 117, 144	0
1	B	400/448 (89%)	0.36	24 (6%) 27 27	31, 60, 116, 162	0
All	All	800/896 (89%)	0.39	42 (5%) 32 32	31, 64, 116, 162	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	ILE	6.5
1	A	252	ALA	6.4
1	B	283	TRP	6.1
1	B	252	ALA	5.4
1	B	406	ILE	5.4
1	B	284	TYR	4.7
1	A	406	ILE	4.7
1	B	282	SER	4.3
1	A	283	TRP	4.3
1	B	253	GLN	4.2
1	B	281	ASN	3.9
1	B	407	LEU	3.8
1	B	344	VAL	3.8
1	A	400	ILE	3.7
1	A	106	GLU	3.3
1	B	472	SER	3.3
1	B	404	THR	3.1
1	B	438	LEU	3.0
1	B	403	CYS	2.9
1	B	323	SER	2.7
1	A	344	VAL	2.7
1	A	324	ASN	2.7
1	A	356	TRP	2.7
1	B	402	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	404	THR	2.6
1	B	436	GLY	2.6
1	B	400	ILE	2.5
1	B	255	ASN	2.5
1	B	471	ALA	2.5
1	A	256	PRO	2.4
1	A	325	PRO	2.4
1	A	284	TYR	2.4
1	B	405	GLU	2.4
1	B	430	THR	2.3
1	B	468	GLN	2.2
1	A	253	GLN	2.2
1	A	402	LYS	2.1
1	A	280	GLN	2.1
1	B	280	GLN	2.1
1	A	405	GLU	2.1
1	A	198	LEU	2.0
1	A	259	PRO	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 oligosaccharides 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.