Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:56 PM EDT

PDB ID	:	1PXZ
Title	:	1.7 Angstrom Crystal Structure of jun a 1, the major allergen from cedar pollen
Authors	:	Czerwinski, E.W.; White, M.A.; Midoro-Horiuti, T.; Brooks, E.G.; Goldblum, R.M.
Deposited on	:	2003-07-07
Resolution	:	1.70 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:

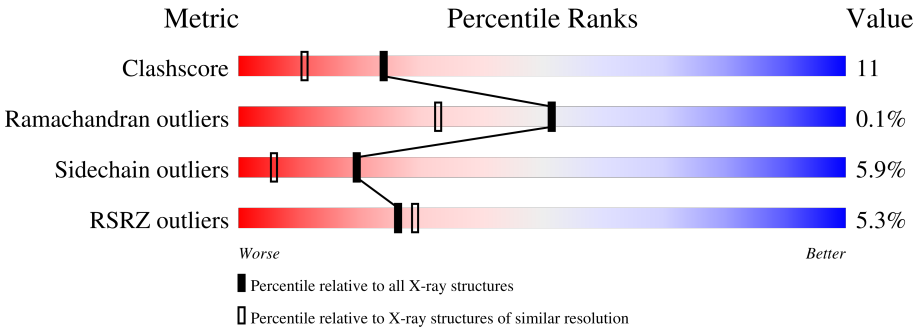
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.70 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))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	346	5% 82% 16% ·
1	B	346	6% 80% 16% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5991 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 Major pollen allergen Jun a 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2645	1641	471	517	16			
1	B	346	Total	C	N	O	S	0	0	0
			2645	1641	471	517	16			

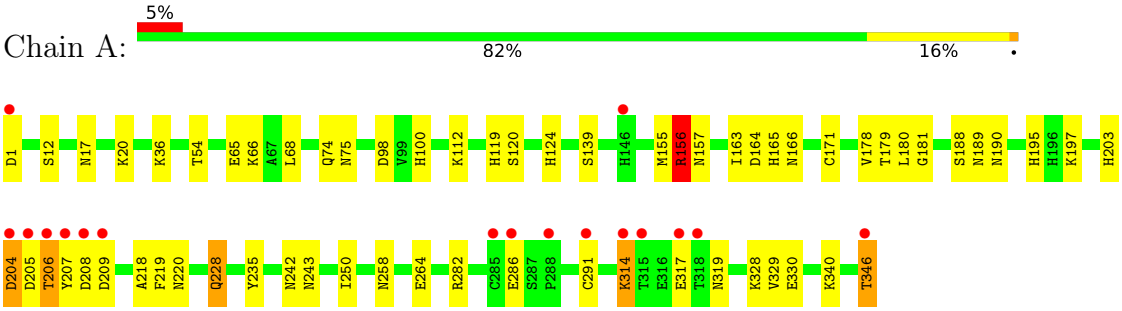
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	342	Total	O	0	0
			342	342		
2	B	359	Total	O	0	0
			359	359		

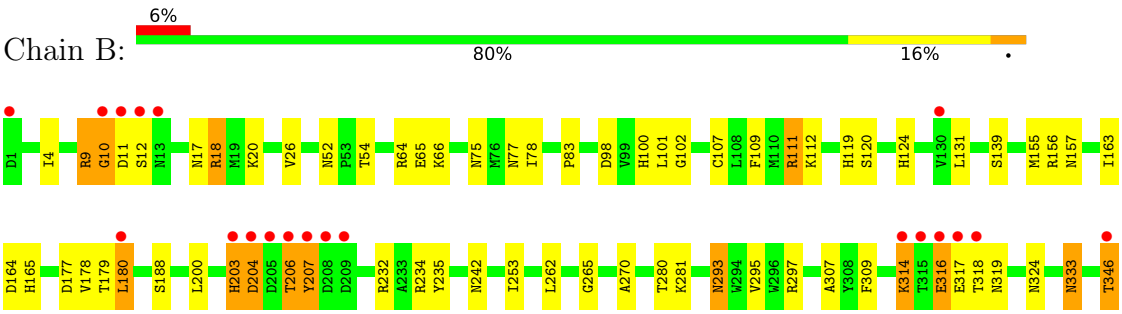
3 Residue-property plots (i)

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: Major pollen allergen Jun a 1



• Molecule 1: Major pollen allergen Jun a 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.64Å 115.00Å 73.53Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	100.00 – 1.70 25.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	86.7 (100.00-1.70) 81.6 (25.29-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 1.70Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.193 , 0.241 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	11.1	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5991	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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	0.90	1/2707 (0.0%)	1.04	3/3677 (0.1%)
1	B	0.90	1/2707 (0.0%)	1.05	6/3677 (0.2%)
All	All	0.90	2/5414 (0.0%)	1.04	9/7354 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	346	THR	C-OXT	41.99	2.03	1.23
1	A	346	THR	C-OXT	41.77	2.02	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	232	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	A	156	ARG	CD-NE-CZ	8.68	135.75	123.60
1	B	18	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	B	309	PHE	CB-CG-CD1	7.77	126.24	120.80
1	B	232	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	156	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	235	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	B	111	ARG	CD-NE-CZ	5.54	131.36	123.60
1	B	64	ARG	CD-NE-CZ	5.48	131.27	123.60

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	2645	0	2515	50	0
1	B	2645	0	2515	64	0
2	A	342	0	0	5	0
2	B	359	0	0	7	0
All	All	5991	0	5030	114	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 11.

All (114) 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:346:THR:OXT	1:A:346:THR:C	2.02	0.98
1:B:346:THR:OXT	1:B:346:THR:C	2.03	0.97
1:B:155:MET:HE3	1:B:178:VAL:HG22	1.63	0.80
1:B:204:ASP:OD2	1:B:207:TYR:HB2	1.82	0.79
1:A:205:ASP:HB3	2:A:423:HOH:O	1.86	0.76
1:A:156:ARG:HH11	1:A:156:ARG:HG2	1.52	0.75
1:B:262:LEU:HD13	1:B:318:THR:HG21	1.68	0.74
1:A:242:ASN:HD21	1:A:330:GLU:H	1.38	0.72
1:B:75:ASN:ND2	1:B:98:ASP:H	1.86	0.72
1:B:111:ARG:HD2	1:B:112:LYS:HZ1	1.56	0.71
1:A:314:LYS:H	1:A:314:LYS:NZ	1.90	0.70
1:A:166:ASN:H	1:A:190:ASN:HD22	1.38	0.70
1:A:54:THR:HG22	2:A:431:HOH:O	1.91	0.70
1:A:12:SER:HB2	1:A:20:LYS:HZ2	1.57	0.69
1:B:203:HIS:HB3	1:B:204:ASP:OD1	1.93	0.69
1:B:111:ARG:HD2	1:B:112:LYS:NZ	2.08	0.69
1:B:293:ASN:H	1:B:293:ASN:HD22	1.42	0.68
1:B:54:THR:HG23	2:B:485:HOH:O	1.93	0.67
1:A:220:ASN:H	1:A:243:ASN:HD22	1.43	0.67
1:B:77:ASN:HD22	1:B:100:HIS:HB2	1.61	0.66
1:A:12:SER:HB2	1:A:20:LYS:NZ	2.11	0.65
1:B:65:GLU:OE1	1:B:139:SER:HB2	1.96	0.64
1:A:166:ASN:H	1:A:190:ASN:ND2	1.96	0.64
1:B:179:THR:HG21	1:B:203:HIS:CG	2.33	0.63
1:A:75:ASN:ND2	1:A:98:ASP:H	1.96	0.63
1:A:190:ASN:H	1:A:220:ASN:HD22	1.46	0.63
1:A:171:CYS:H	1:A:195:HIS:HD2	1.46	0.62
1:A:112:LYS:HZ3	1:A:156:ARG:HH12	1.49	0.60
1:B:200:LEU:HD23	1:B:203:HIS:CE1	2.36	0.60
1:B:293:ASN:H	1:B:293:ASN:ND2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:MET:HE2	1:A:163:ILE:HD11	1.85	0.59
1:A:204:ASP:HB2	1:A:206:THR:HG23	1.85	0.58
1:A:314:LYS:H	1:A:314:LYS:CE	2.16	0.58
1:A:204:ASP:OD1	1:A:207:TYR:HB2	2.04	0.58
1:B:281:LYS:HD2	2:B:644:HOH:O	2.05	0.57
1:A:190:ASN:H	1:A:220:ASN:ND2	2.01	0.57
1:B:324:ASN:HB3	2:B:532:HOH:O	2.04	0.57
1:B:75:ASN:HD22	1:B:98:ASP:H	1.51	0.57
1:A:171:CYS:H	1:A:195:HIS:CD2	2.22	0.56
1:B:204:ASP:O	1:B:234:ARG:HD3	2.05	0.56
1:A:155:MET:HE3	1:A:178:VAL:HG22	1.86	0.56
1:B:180:LEU:HA	1:B:207:TYR:HE2	1.71	0.55
1:B:112:LYS:HZ1	1:B:156:ARG:NH2	2.06	0.53
1:B:180:LEU:HA	1:B:207:TYR:CE2	2.43	0.53
1:B:314:LYS:HE2	1:B:314:LYS:N	2.23	0.53
1:B:180:LEU:HD23	1:B:180:LEU:O	2.09	0.53
1:B:100:HIS:HD2	1:B:124:HIS:NE2	2.07	0.53
1:A:220:ASN:H	1:A:243:ASN:ND2	2.06	0.52
1:A:179:THR:HG22	1:A:203:HIS:HB2	1.92	0.51
1:A:346:THR:OXT	1:A:346:THR:O	2.28	0.51
1:B:333:ASN:HD22	1:B:333:ASN:N	2.09	0.51
1:B:346:THR:OXT	1:B:346:THR:O	2.28	0.51
1:A:100:HIS:HD2	1:A:124:HIS:NE2	2.09	0.50
1:B:295:VAL:CG2	1:B:314:LYS:HE3	2.41	0.50
1:B:234:ARG:O	1:B:235:TYR:HB2	2.11	0.50
1:B:179:THR:HG21	1:B:203:HIS:ND1	2.27	0.49
1:A:75:ASN:HD22	1:A:98:ASP:H	1.59	0.49
1:B:155:MET:HE3	1:B:178:VAL:CG2	2.40	0.49
1:A:179:THR:CG2	1:A:203:HIS:HB2	2.43	0.49
1:A:180:LEU:HD12	1:A:207:TYR:CZ	2.48	0.48
1:A:264:GLU:HG2	1:A:329:VAL:HG11	1.94	0.48
1:B:179:THR:HG21	1:B:203:HIS:CB	2.43	0.48
1:B:157:ASN:HB2	1:B:180:LEU:HD23	1.96	0.47
1:B:155:MET:HE1	1:B:163:ILE:HD11	1.96	0.47
1:B:11:ASP:OD1	1:B:12:SER:N	2.48	0.46
1:B:119:HIS:HA	1:B:164:ASP:O	2.16	0.46
1:B:9:ARG:O	1:B:10:GLY:O	2.33	0.46
1:B:297:ARG:HH22	1:B:316:GLU:HB3	1.80	0.46
1:B:157:ASN:ND2	2:B:524:HOH:O	2.49	0.46
1:B:314:LYS:HE2	1:B:314:LYS:H	1.80	0.46
1:A:20:LYS:NZ	2:A:482:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:HA2	2:A:688:HOH:O	2.15	0.45
1:B:319:ASN:HB2	2:B:572:HOH:O	2.16	0.45
1:A:66:LYS:HE2	1:A:68:LEU:HD21	1.98	0.45
1:A:155:MET:CE	1:A:178:VAL:HG22	2.46	0.45
1:A:164:ASP:HA	1:A:188:SER:O	2.17	0.45
1:B:164:ASP:HA	1:B:188:SER:O	2.17	0.45
1:A:228:GLN:NE2	1:A:250:ILE:HD12	2.33	0.44
1:A:258:ASN:ND2	2:A:393:HOH:O	2.49	0.44
1:A:120:SER:HA	1:A:165:HIS:O	2.17	0.44
1:B:297:ARG:NH1	1:B:314:LYS:O	2.50	0.44
1:B:177:ASP:OD2	1:B:203:HIS:HE1	2.00	0.44
1:B:180:LEU:HD12	1:B:207:TYR:CZ	2.52	0.44
1:B:120:SER:HA	1:B:165:HIS:O	2.18	0.44
1:B:18:ARG:NH2	2:B:650:HOH:O	2.50	0.43
1:A:165:HIS:HA	1:A:189:ASN:O	2.19	0.43
1:A:282:ARG:HH11	1:A:282:ARG:HD2	1.66	0.43
1:B:180:LEU:HD12	1:B:207:TYR:CE2	2.53	0.43
1:B:295:VAL:HG22	1:B:314:LYS:HE3	1.98	0.43
1:B:157:ASN:HD22	1:B:180:LEU:HD21	1.84	0.43
1:B:179:THR:HG21	1:B:203:HIS:HB2	2.01	0.43
1:B:270:ALA:HB2	1:B:307:ALA:HB2	2.00	0.43
1:A:207:TYR:CE2	1:A:209:ASP:HB2	2.54	0.42
1:A:119:HIS:HA	1:A:164:ASP:O	2.18	0.42
1:A:195:HIS:HE1	1:A:197:LYS:O	2.02	0.42
1:A:188:SER:HA	1:A:218:ALA:O	2.19	0.42
1:B:155:MET:CE	1:B:163:ILE:HD11	2.49	0.42
1:B:253:ILE:O	1:B:280:THR:HA	2.20	0.42
1:A:180:LEU:O	1:A:180:LEU:HG	2.19	0.42
1:B:4:ILE:HD11	1:B:26:VAL:HG22	2.00	0.42
1:A:155:MET:CE	1:A:163:ILE:HD11	2.49	0.42
1:B:178:VAL:O	1:B:179:THR:HG23	2.19	0.42
1:B:78:ILE:HB	1:B:101:LEU:HD23	2.02	0.42
1:A:228:GLN:CD	1:A:250:ILE:HD12	2.40	0.41
1:B:204:ASP:HB2	1:B:206:THR:OG1	2.21	0.41
1:A:219:PHE:HA	1:A:242:ASN:O	2.21	0.41
1:A:314:LYS:H	1:A:314:LYS:HZ3	1.66	0.41
1:B:242:ASN:HA	1:B:265:GLY:O	2.21	0.41
1:B:83:PRO:HB3	1:B:109:PHE:CE1	2.56	0.40
1:B:324:ASN:ND2	2:B:646:HOH:O	2.50	0.40
1:A:74:GLN:HG3	1:A:75:ASN:O	2.22	0.40
1:B:112:LYS:NZ	1:B:156:ARG:NH2	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASN:HB2	1:B:180:LEU:CD2	2.52	0.40
1:B:102:GLY:HA2	1:B:107:CYS:SG	2.61	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	344/346 (99%)	330 (96%)	14 (4%)	0	100 100
1	B	344/346 (99%)	328 (95%)	15 (4%)	1 (0%)	41 24
All	All	688/692 (99%)	658 (96%)	29 (4%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	GLY

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	289/289 (100%)	271 (94%)	18 (6%)	18 5
1	B	289/289 (100%)	273 (94%)	16 (6%)	21 7
All	All	578/578 (100%)	544 (94%)	34 (6%)	19 6

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	17	ASN
1	A	36	LYS
1	A	65	GLU
1	A	139	SER
1	A	156	ARG
1	A	157	ASN
1	A	204	ASP
1	A	206	THR
1	A	208	ASP
1	A	228	GLN
1	A	286	GLU
1	A	291	CYS
1	A	314	LYS
1	A	317	GLU
1	A	319	ASN
1	A	328	LYS
1	A	340	LYS
1	B	9	ARG
1	B	17	ASN
1	B	20	LYS
1	B	52	ASN
1	B	66	LYS
1	B	131	LEU
1	B	180	LEU
1	B	203	HIS
1	B	204	ASP
1	B	206	THR
1	B	207	TYR
1	B	293	ASN
1	B	314	LYS
1	B	316	GLU
1	B	317	GLU
1	B	333	ASN

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

Mol	Chain	Res	Type
1	A	17	ASN
1	A	75	ASN
1	A	100	HIS

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Mol	Chain	Res	Type
1	A	190	ASN
1	A	195	HIS
1	A	196	HIS
1	A	220	ASN
1	A	228	GLN
1	A	242	ASN
1	A	243	ASN
1	A	249	ASN
1	A	258	ASN
1	A	293	ASN
1	A	319	ASN
1	A	324	ASN
1	B	17	ASN
1	B	52	ASN
1	B	74	GLN
1	B	75	ASN
1	B	77	ASN
1	B	100	HIS
1	B	157	ASN
1	B	225	ASN
1	B	258	ASN
1	B	293	ASN
1	B	333	ASN

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 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	346/346 (100%)	-0.02	17 (4%)	29	33	6, 14, 39, 91	0
1	B	346/346 (100%)	0.11	20 (5%)	23	25	7, 15, 50, 116	0
All	All	692/692 (100%)	0.05	37 (5%)	26	29	6, 15, 48, 116	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	TYR	12.5
1	B	12	SER	11.2
1	B	205	ASP	10.2
1	B	11	ASP	9.5
1	B	206	THR	7.5
1	A	207	TYR	7.1
1	A	206	THR	6.7
1	B	315	THR	6.2
1	B	318	THR	5.4
1	B	209	ASP	5.1
1	A	315	THR	5.0
1	A	286	GLU	4.9
1	B	204	ASP	4.8
1	B	317	GLU	4.7
1	A	205	ASP	4.6
1	A	204	ASP	4.3
1	B	10	GLY	4.2
1	B	208	ASP	4.0
1	A	209	ASP	3.9
1	B	316	GLU	3.7
1	B	314	LYS	3.5
1	A	146	HIS	3.4
1	A	317	GLU	3.2
1	A	285	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	318	THR	3.0
1	A	346	THR	2.9
1	B	13	ASN	2.9
1	B	130	VAL	2.9
1	B	180	LEU	2.9
1	B	346	THR	2.7
1	B	203	HIS	2.7
1	A	1	ASP	2.7
1	B	1	ASP	2.6
1	A	208	ASP	2.5
1	A	291	CYS	2.5
1	A	314	LYS	2.2
1	A	288	PRO	2.1

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.