Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WXZ
Title : CRYSTAL STRUCTURE OF RAT ANGIOTENSINOGEN IN C2 SPACE GROUP
Authors : Zhou, A.; Wei, Z.; Carrell, R.W.; Read, R.J.
Deposited on : 2009-11-11
Resolution : 2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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.
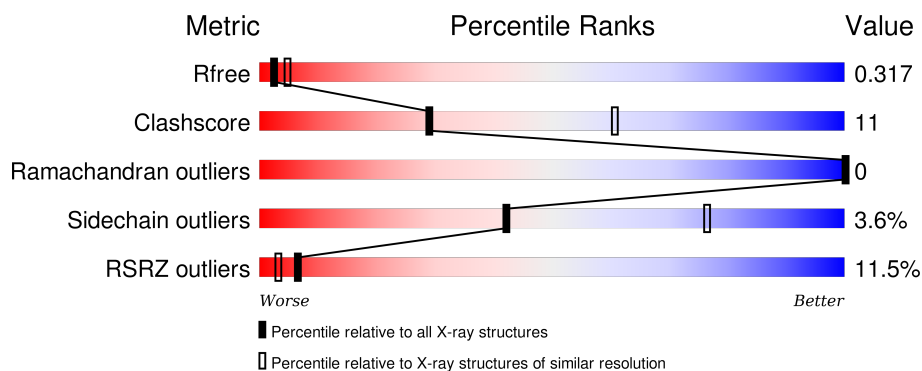
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	453	8% / 70% / 22% / · 7%
2	C	453	13% / 70% / 21% / 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6473 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 ANGIOTENSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total 3266	C 2097	N 551	O 608	S 10	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	VAL	MET	CONFLICT	UNP P01015

- Molecule 2 is a protein called ANGIOTENSINOGEN.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	413	Total 3207	C 2062	N 540	O 594	S 11	0	2	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: ANGIOTENSINOGEN
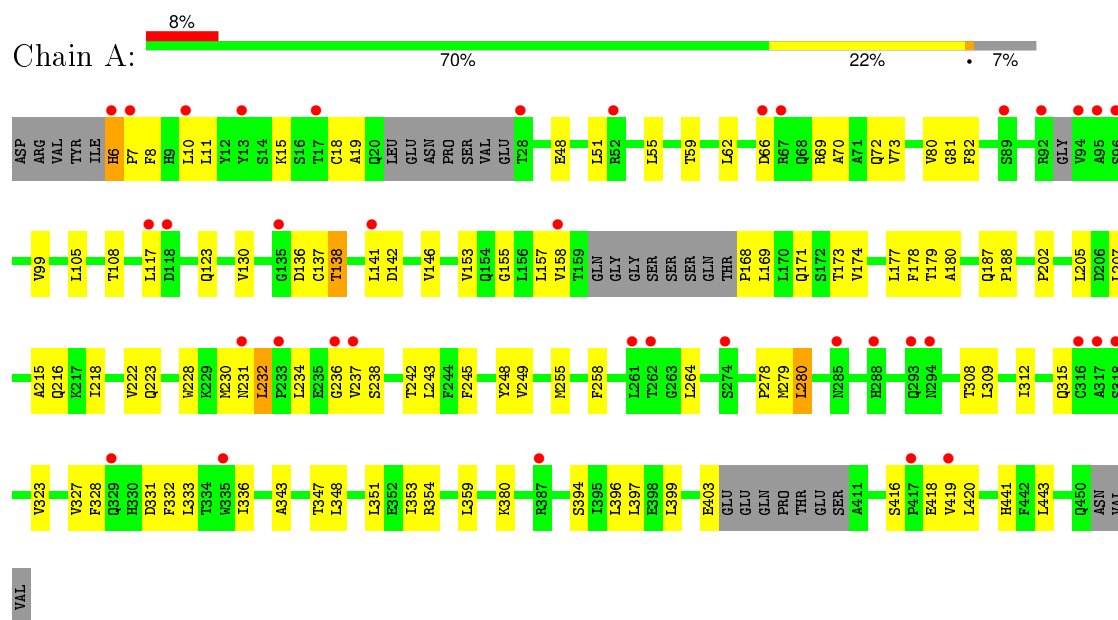
- Molecule 2: ANGIOTENSINOGEN
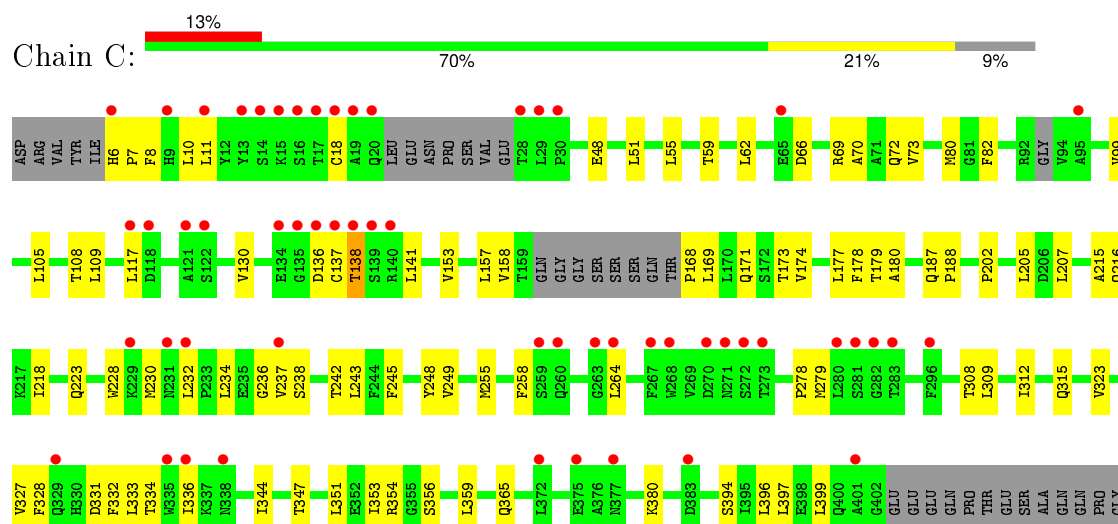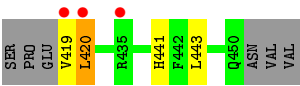
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.50Å 49.54Å 150.28Å 90.00° 90.84° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 46.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.80) 98.2 (46.31-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0099	Depositor
R, R_{free}	0.282 , 0.310 0.284 , 0.317	Depositor DCC
R_{free} test set	1212 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.5	EDS
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 23701 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6473	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.33	0/3341	0.51	0/4547
2	C	0.31	0/3283	0.50	0/4466
All	All	0.32	0/6624	0.50	0/9013

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 (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	3266	0	3292	78	0
2	C	3207	0	3241	72	0
All	All	6473	0	6533	148	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 (148) 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)
2:C:234:LEU:HD13	2:C:237:VAL:HG21	1.36	1.08
1:A:416:SER:O	1:A:419:VAL:HG23	1.54	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ALA:HB2	1:A:234:LEU:HD22	1.39	1.04
2:C:99:VAL:HG21	2:C:353:ILE:HG21	1.46	0.94
1:A:99:VAL:HG21	1:A:353:ILE:HG21	1.47	0.94
2:C:99:VAL:HG21	2:C:353:ILE:CG2	1.99	0.92
1:A:99:VAL:CG2	1:A:353:ILE:HG21	2.00	0.91
1:A:99:VAL:HG21	1:A:353:ILE:CG2	2.01	0.91
2:C:99:VAL:CG2	2:C:353:ILE:HG21	2.00	0.89
1:A:215:ALA:HB2	1:A:234:LEU:CD2	2.09	0.82
2:C:234:LEU:HD13	2:C:237:VAL:CG2	2.09	0.81
1:A:130:VAL:HG21	1:A:141:LEU:HD21	1.65	0.79
1:A:215:ALA:CB	1:A:234:LEU:HD22	2.13	0.77
1:A:351:LEU:HD12	1:A:399:LEU:HD13	1.66	0.77
2:C:351:LEU:HD12	2:C:399:LEU:HD13	1.67	0.77
2:C:130:VAL:HG21	2:C:141:LEU:HD21	1.68	0.76
1:A:234:LEU:HD23	1:A:237:VAL:HG21	1.68	0.75
2:C:420:LEU:HD22	2:C:420:LEU:O	1.87	0.74
1:A:416:SER:O	1:A:419:VAL:CG2	2.34	0.74
2:C:234:LEU:CD1	2:C:237:VAL:HG21	2.16	0.73
1:A:123:GLN:HE21	2:C:334:THR:HG21	1.56	0.70
2:C:157:LEU:HD22	2:C:441:HIS:CG	2.29	0.68
1:A:157:LEU:HD22	1:A:441:HIS:CG	2.29	0.67
2:C:99:VAL:CG2	2:C:353:ILE:CG2	2.68	0.64
1:A:99:VAL:CG2	1:A:353:ILE:CG2	2.68	0.63
1:A:123:GLN:NE2	2:C:334:THR:HG21	2.14	0.62
2:C:205:LEU:HD21	2:C:207:LEU:HD21	1.82	0.62
2:C:99:VAL:HG21	2:C:353:ILE:HG22	1.81	0.61
1:A:205:LEU:HD21	1:A:207:LEU:HD21	1.82	0.61
2:C:6:HIS:N	2:C:7:PRO:CD	2.64	0.61
2:C:351:LEU:CD1	2:C:399:LEU:HD13	2.31	0.60
1:A:6:HIS:N	1:A:7:PRO:CD	2.64	0.60
1:A:99:VAL:HG21	1:A:353:ILE:HG22	1.84	0.59
1:A:105:LEU:HD21	1:A:359:LEU:HD13	1.84	0.59
2:C:105:LEU:HD21	2:C:359:LEU:HD13	1.84	0.58
1:A:309:LEU:HD22	1:A:399:LEU:HD21	1.86	0.58
2:C:80:MET:HE3	2:C:109:LEU:CD1	2.33	0.58
1:A:179:THR:HG22	1:A:243:LEU:HD23	1.85	0.58
1:A:351:LEU:CD1	1:A:399:LEU:HD13	2.32	0.57
2:C:105:LEU:HD21	2:C:359:LEU:CD1	2.35	0.57
2:C:179:THR:HG22	2:C:243:LEU:HD23	1.87	0.56
2:C:309:LEU:HD22	2:C:399:LEU:HD21	1.88	0.56
1:A:105:LEU:HD21	1:A:359:LEU:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:236:GLY:O	2:C:237:VAL:HG23	2.08	0.54
2:C:80:MET:CE	2:C:109:LEU:CD1	2.86	0.54
2:C:80:MET:HE3	2:C:109:LEU:HD11	1.89	0.54
1:A:10:LEU:HB3	1:A:69:ARG:HG3	1.89	0.54
1:A:178:PHE:CZ	1:A:218:ILE:HG23	2.43	0.53
2:C:55:LEU:O	2:C:59:THR:HG23	2.09	0.53
2:C:420:LEU:HD13	2:C:420:LEU:H	1.74	0.53
2:C:157:LEU:HD22	2:C:441:HIS:ND1	2.23	0.53
1:A:157:LEU:HD22	1:A:441:HIS:ND1	2.24	0.53
1:A:230:MET:HE2	1:A:394:SER:HB3	1.91	0.53
2:C:10:LEU:HB3	2:C:69:ARG:HG3	1.90	0.52
1:A:108:THR:HG23	1:A:245:PHE:CE2	2.44	0.52
1:A:280:LEU:CD2	1:A:348:LEU:HD21	2.40	0.52
2:C:158:VAL:O	2:C:158:VAL:HG23	2.09	0.52
1:A:343:ALA:HB3	1:A:418:GLU:O	2.10	0.51
2:C:237:VAL:HG12	2:C:238:SER:O	2.10	0.51
1:A:237:VAL:HG12	1:A:238:SER:O	2.10	0.51
1:A:55:LEU:O	1:A:59:THR:HG23	2.11	0.51
1:A:153:VAL:HG12	1:A:441:HIS:CE1	2.46	0.50
2:C:178:PHE:CZ	2:C:218:ILE:HG23	2.46	0.50
2:C:108:THR:HG23	2:C:245:PHE:CE2	2.46	0.50
1:A:180:ALA:HB2	1:A:242:THR:HA	1.94	0.49
1:A:236:GLY:O	1:A:237:VAL:HG23	2.13	0.49
1:A:215:ALA:CB	1:A:234:LEU:CD2	2.82	0.49
2:C:174:VAL:HG22	2:C:248:TYR:HB2	1.94	0.48
1:A:280:LEU:CD2	1:A:348:LEU:CD2	2.91	0.48
1:A:264:LEU:HD22	1:A:278:PRO:HD3	1.95	0.48
1:A:333:LEU:HB3	1:A:336:ILE:HD12	1.96	0.48
2:C:8:PHE:HB3	2:C:11:LEU:HD12	1.96	0.48
2:C:6:HIS:N	2:C:7:PRO:HD3	2.28	0.48
2:C:230:MET:HE2	2:C:394:SER:HB3	1.95	0.48
1:A:168:PRO:O	1:A:169:LEU:HD12	2.13	0.48
2:C:153:VAL:HG12	2:C:441:HIS:CE1	2.49	0.47
2:C:232:LEU:HD22	2:C:356:SER:HB2	1.96	0.47
2:C:279:MET:HE3	2:C:347:THR:HG22	1.95	0.47
2:C:177:LEU:O	2:C:202:PRO:HA	2.15	0.47
1:A:177:LEU:O	1:A:202:PRO:HA	2.15	0.47
1:A:10:LEU:CB	1:A:69:ARG:HG3	2.44	0.47
1:A:6:HIS:N	1:A:7:PRO:HD3	2.29	0.47
2:C:180:ALA:HB2	2:C:242:THR:HA	1.95	0.47
1:A:158:VAL:HG23	1:A:158:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:LEU:HD22	2:C:66:ASP:HB3	1.97	0.46
2:C:323:VAL:O	2:C:327:VAL:HG22	2.16	0.46
1:A:231:ASN:C	1:A:232:LEU:HD13	2.36	0.46
1:A:136:ASP:OD1	1:A:138:THR:HG23	2.15	0.46
1:A:174:VAL:HG22	1:A:248:TYR:HB2	1.97	0.46
1:A:279:MET:HE3	1:A:347:THR:HG22	1.97	0.46
1:A:8:PHE:HB3	1:A:11:LEU:HD12	1.98	0.46
1:A:82:PHE:CD2	1:A:331:ASP:HA	2.52	0.45
2:C:10:LEU:CB	2:C:69:ARG:HG3	2.45	0.45
1:A:173:THR:HG22	1:A:249:VAL:HG22	1.98	0.45
2:C:117:LEU:HD21	2:C:380:LYS:HG3	1.98	0.45
2:C:264:LEU:HD22	2:C:278:PRO:HD3	1.98	0.45
1:A:158:VAL:HG11	1:A:171:GLN:HB3	1.99	0.45
2:C:82:PHE:CD2	2:C:331:ASP:HA	2.51	0.45
1:A:309:LEU:HD22	1:A:399:LEU:CD2	2.47	0.45
1:A:230:MET:CE	1:A:394:SER:HB3	2.47	0.45
1:A:62:LEU:HD22	1:A:66:ASP:HB3	1.99	0.45
2:C:333:LEU:HB3	2:C:336:ILE:HD12	1.99	0.45
2:C:158:VAL:HG11	2:C:171:GLN:HB3	1.99	0.44
2:C:354:ARG:CG	2:C:396:LEU:HD13	2.48	0.44
1:A:234:LEU:HD23	1:A:237:VAL:CG2	2.43	0.43
1:A:48:GLU:HA	1:A:51:LEU:HD12	1.99	0.43
1:A:80:VAL:HG13	1:A:81:GLY:N	2.33	0.43
2:C:168:PRO:O	2:C:169:LEU:HD12	2.18	0.43
2:C:173:THR:HG22	2:C:249:VAL:HG22	2.00	0.43
2:C:309:LEU:HD22	2:C:399:LEU:CD2	2.49	0.42
2:C:230:MET:CE	2:C:394:SER:HB3	2.49	0.42
2:C:10:LEU:HD12	2:C:72:GLN:NE2	2.34	0.42
1:A:327:VAL:HG23	1:A:328:PHE:N	2.34	0.42
1:A:142:ASP:O	1:A:146:VAL:HG23	2.20	0.42
2:C:136:ASP:OD1	2:C:138:THR:HG23	2.19	0.42
2:C:80:MET:HE2	2:C:109:LEU:HD13	2.01	0.42
1:A:323:VAL:O	1:A:327:VAL:HG22	2.19	0.42
2:C:344:ILE:HG12	2:C:420:LEU:CD2	2.49	0.42
1:A:230:MET:HB3	1:A:232:LEU:HD11	2.01	0.42
1:A:354:ARG:CG	1:A:396:LEU:HD13	2.49	0.42
2:C:187:GLN:N	2:C:188:PRO:CD	2.83	0.42
1:A:218:ILE:O	1:A:222:VAL:HG23	2.20	0.41
2:C:178:PHE:O	2:C:243:LEU:HD22	2.21	0.41
1:A:117:LEU:HD21	1:A:380:LYS:HG3	2.02	0.41
1:A:59:THR:HG22	1:A:155:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:255:MET:HE2	2:C:258:PHE:CD2	2.55	0.41
2:C:312:ILE:N	2:C:312:ILE:HD12	2.36	0.41
1:A:10:LEU:HD12	1:A:72:GLN:NE2	2.36	0.41
2:C:48:GLU:HA	2:C:51:LEU:HD12	2.02	0.41
1:A:243:LEU:HD13	1:A:243:LEU:C	2.41	0.41
1:A:82:PHE:CD1	1:A:328:PHE:O	2.74	0.41
2:C:70:ALA:HA	2:C:73:VAL:HG12	2.03	0.41
1:A:187:GLN:N	1:A:188:PRO:CD	2.84	0.41
1:A:397:LEU:CD2	1:A:399:LEU:HD12	2.51	0.41
1:A:280:LEU:HD21	1:A:348:LEU:HD21	2.03	0.41
2:C:327:VAL:HG23	2:C:328:PHE:N	2.36	0.41
1:A:70:ALA:HA	1:A:73:VAL:HG12	2.03	0.41
2:C:443:LEU:HD12	2:C:443:LEU:C	2.41	0.41
1:A:443:LEU:C	1:A:443:LEU:HD12	2.40	0.41
1:A:178:PHE:O	1:A:243:LEU:HD22	2.21	0.41
2:C:243:LEU:C	2:C:243:LEU:HD13	2.41	0.41
2:C:397:LEU:CD2	2:C:399:LEU:HD12	2.51	0.40
2:C:215:ALA:HB2	2:C:234:LEU:HD12	2.03	0.40
2:C:397:LEU:CD2	2:C:399:LEU:CD1	2.99	0.40
1:A:255:MET:HE2	1:A:258:PHE:CD2	2.57	0.40
1:A:15:LYS:O	1:A:19:ALA:HB2	2.21	0.40
2:C:80:MET:CE	2:C:109:LEU:HD13	2.51	0.40
1:A:312:ILE:HD12	1:A:312:ILE:N	2.35	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	413/453 (91%)	391 (95%)	22 (5%)	0	100	100
2	C	405/453 (89%)	383 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	818/906 (90%)	774 (95%)	44 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	364/391 (93%)	350 (96%)	14 (4%)	40	74
2	C	358/391 (92%)	346 (97%)	12 (3%)	44	78
All	All	722/782 (92%)	696 (96%)	26 (4%)	42	76

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	18	CYS
1	A	137	CYS
1	A	138	THR
1	A	216	GLN
1	A	223	GLN
1	A	228	TRP
1	A	232	LEU
1	A	280	LEU
1	A	308	THR
1	A	315	GLN
1	A	332	PHE
1	A	403	GLU
1	A	420	LEU
2	C	18	CYS
2	C	137	CYS
2	C	138	THR
2	C	216	GLN
2	C	223	GLN
2	C	228	TRP

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type
2	C	308	THR
2	C	315	GLN
2	C	332	PHE
2	C	365	GLN
2	C	419	VAL
2	C	420	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	422/453 (93%)	0.55	38 (9%)	12	6	27, 55, 93, 117	7 (1%)
2	C	413/453 (91%)	0.77	58 (14%)	4	2	39, 62, 94, 117	6 (1%)
All	All	835/906 (92%)	0.66	96 (11%)	6	3	27, 60, 93, 117	13 (1%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	281	SER	5.6
2	C	28	THR	5.3
2	C	118	ASP	5.2
1	A	293	GLN	5.0
1	A	17	THR	4.9
1	A	329	GLN	4.8
2	C	135	GLY	4.8
1	A	6	HIS	4.7
1	A	294	ASN	4.6
1	A	95	ALA	4.5
2	C	29	LEU	4.4
1	A	67	ARG	4.4
2	C	13	TYR	4.3
2	C	138	THR	4.1
1	A	96	SER	4.1
2	C	282	GLY	4.0
2	C	338	ASN	3.9
2	C	134	GLU	3.9
2	C	117	LEU	3.9
2	C	268	TRP	3.9
2	C	271	ASN	3.8
1	A	231	ASN	3.7
2	C	95	ALA	3.6
2	C	270	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	233	PRO	3.5
2	C	283	THR	3.5
2	C	335	TRP	3.4
2	C	18	CYS	3.3
1	A	318	SER	3.3
2	C	137	CYS	3.3
2	C	229	LYS	3.3
2	C	329	GLN	3.3
2	C	19	ALA	3.2
1	A	118	ASP	3.2
2	C	383[A]	ASP	3.1
2	C	16	SER	3.1
2	C	65	GLU	3.1
2	C	260	GLN	3.0
2	C	296	PHE	3.0
2	C	280	LEU	3.0
2	C	17	THR	3.0
2	C	231	ASN	2.9
2	C	267	PHE	2.9
2	C	20	GLN	2.9
2	C	435	ARG	2.9
1	A	316	CYS	2.9
1	A	419	VAL	2.7
1	A	387	ARG	2.7
1	A	52	ARG	2.7
1	A	274	SER	2.7
2	C	372	LEU	2.7
1	A	261	LEU	2.6
2	C	420	LEU	2.6
1	A	92	ARG	2.6
2	C	9	HIS	2.5
2	C	14	SER	2.5
1	A	7	PRO	2.5
2	C	237	VAL	2.5
2	C	419	VAL	2.5
2	C	136	ASP	2.5
1	A	66	ASP	2.5
2	C	15	LYS	2.5
2	C	11	LEU	2.5
2	C	264	LEU	2.4
1	A	89	SER	2.4
1	A	317	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	417	PRO	2.4
1	A	10	LEU	2.4
1	A	285	ASN	2.3
1	A	335	TRP	2.3
1	A	13	TYR	2.3
2	C	273	THR	2.3
2	C	121	ALA	2.2
2	C	6	HIS	2.2
2	C	375	GLU	2.2
1	A	288	HIS	2.2
1	A	237	VAL	2.2
2	C	401	ALA	2.2
2	C	139	SER	2.2
1	A	94	VAL	2.1
1	A	141	LEU	2.1
2	C	377	ASN	2.1
2	C	259	SER	2.1
1	A	117	LEU	2.1
2	C	140	ARG	2.1
2	C	336	ILE	2.1
2	C	232	LEU	2.1
1	A	135	GLY	2.1
1	A	236	GLY	2.1
1	A	28	THR	2.1
2	C	263	GLY	2.0
1	A	158	VAL	2.0
2	C	272	SER	2.0
1	A	262	THR	2.0
2	C	30	PRO	2.0
2	C	122	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 carbohydrates 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.