Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 08:19 AM EDT

PDB ID	:	2WXX
Title	:	Crystal structure of mouse angiotensinogen in the oxidised form
Authors	:	Zhou, A.; Wei, Z.; Carrell, R.W.; Read, R.J.
Deposited on	:	2009-11-11
Resolution	:	2.95 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 (i) 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 (1)) were used in the production of this report:

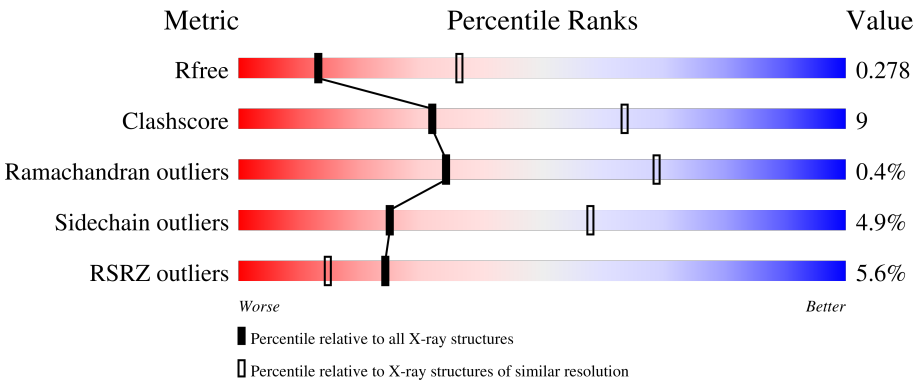
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	453	2% 71% 18% • 9%
1	B	453	4% 75% 18% • 6%
1	C	453	3% 71% 20% • 7%
1	D	453	11% 73% 17% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12945 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
			Total	C	N	O	S			
1	A	412	3181	2036	535	600	10	0	1	0
1	B	428	3314	2117	558	629	10	0	2	0
1	C	422	3274	2095	550	619	10	0	3	0
1	D	411	3176	2036	533	597	10	0	2	0

There are 20 discrepancies between the modelled and reference sequences:

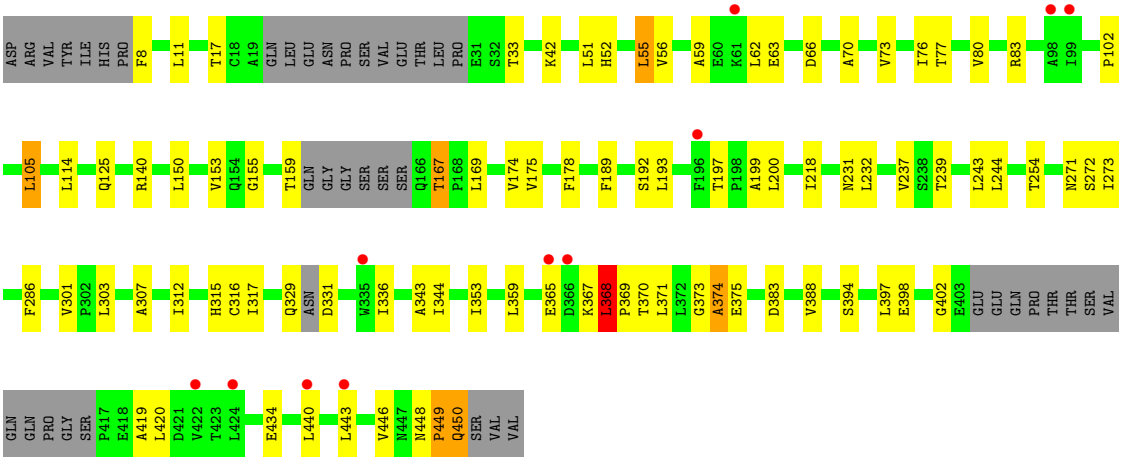
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	THR	ALA	conflict	UNP P11859
A	174	VAL	MET	conflict	UNP P11859
A	317	ILE	THR	conflict	UNP P11859
A	329	GLN	ARG	conflict	UNP P11859
A	379	ASN	SER	conflict	UNP P11859
B	77	THR	ALA	conflict	UNP P11859
B	174	VAL	MET	conflict	UNP P11859
B	317	ILE	THR	conflict	UNP P11859
B	329	GLN	ARG	conflict	UNP P11859
B	379	ASN	SER	conflict	UNP P11859
C	77	THR	ALA	conflict	UNP P11859
C	174	VAL	MET	conflict	UNP P11859
C	317	ILE	THR	conflict	UNP P11859
C	329	GLN	ARG	conflict	UNP P11859
C	379	ASN	SER	conflict	UNP P11859
D	77	THR	ALA	conflict	UNP P11859
D	174	VAL	MET	conflict	UNP P11859
D	317	ILE	THR	conflict	UNP P11859
D	329	GLN	ARG	conflict	UNP P11859
D	379	ASN	SER	conflict	UNP P11859

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.

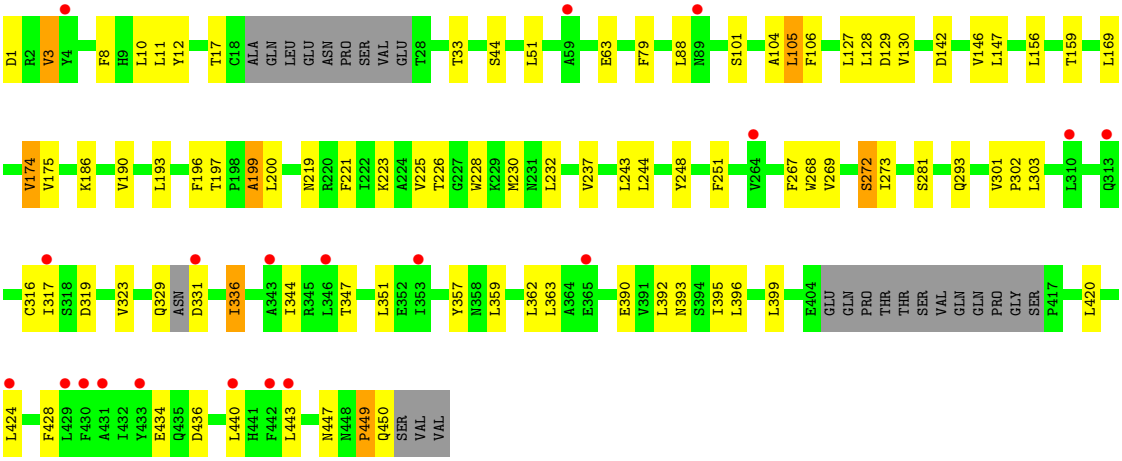
• Molecule 1: ANGIOTENSINOGEN

Chain A:



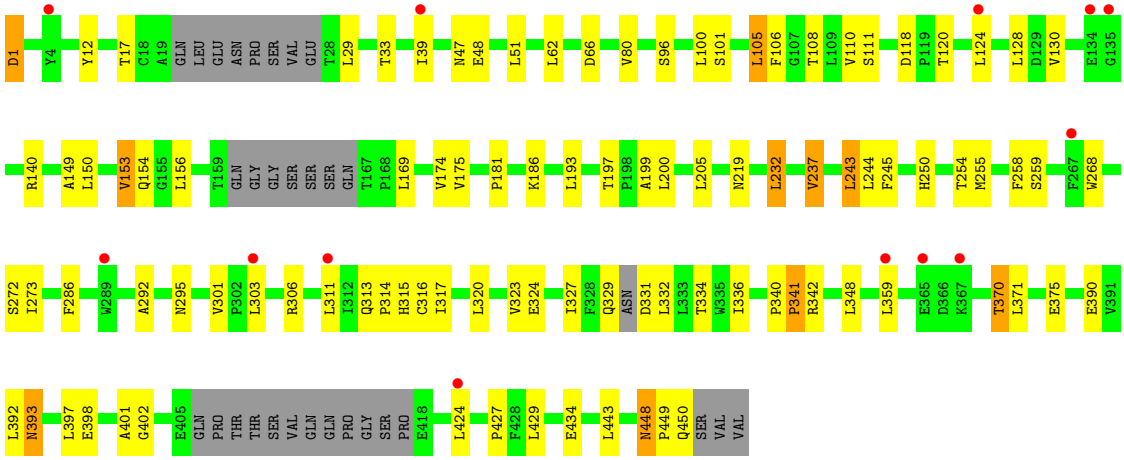
• Molecule 1: ANGIOTENSINOGEN

Chain B:



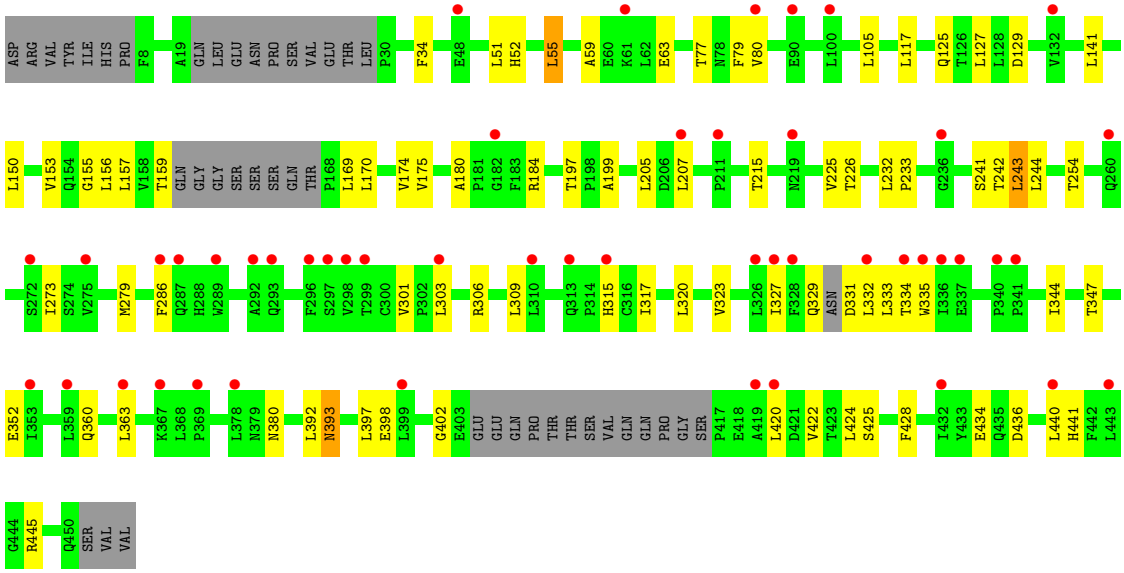
• Molecule 1: ANGIOTENSINOGEN

Chain C:



- Molecule 1: ANGIOTENSINOGEN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	95.37Å 99.42Å 425.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	213.20 – 2.95 68.82 – 2.95	Depositor EDS
% Data completeness (in resolution range)	84.5 (213.20-2.95) 84.5 (68.82-2.95)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.5.0099	Depositor
R, R_{free}	0.223 , 0.271 0.230 , 0.278	Depositor DCC
R_{free} test set	1850 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	76.7	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.055 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12945	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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 (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	0.40	1/3251 (0.0%)	0.54	1/4427 (0.0%)
1	B	0.38	0/3392	0.56	0/4621
1	C	0.34	0/3353	0.50	0/4567
1	D	0.31	0/3250	0.47	0/4424
All	All	0.36	1/13246 (0.0%)	0.52	1/18039 (0.0%)

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	2	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	5	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	THR	CB-OG1	5.40	1.54	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	368	LEU	CA-CB-CG	-5.03	103.73	115.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	167	THR	CB

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Mol	Chain	Res	Type	Atom
1	A	327	ILE	CB
1	B	327	ILE	CB
1	C	327	ILE	CB
1	D	327	ILE	CB

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	3181	0	3179	66	0
1	B	3314	0	3308	56	0
1	C	3274	0	3261	67	0
1	D	3176	0	3173	46	0
All	All	12945	0	12921	230	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 9.

All (230) 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:367:LYS:C	1:A:368:LEU:HD23	1.50	1.29
1:A:371:LEU:HD23	1:A:371:LEU:O	1.48	1.12
1:A:367:LYS:O	1:A:368:LEU:HD23	1.62	1.00
1:C:448:ASN:C	1:C:448:ASN:HD22	1.66	0.97
1:C:193:LEU:HD23	1:C:200:LEU:HD11	1.47	0.94
1:C:311:LEU:HD13	1:C:424:LEU:HD11	1.49	0.91
1:B:440:LEU:HD13	1:B:443:LEU:HD23	1.58	0.86
1:D:333:LEU:HD11	1:D:440:LEU:HD11	1.54	0.86
1:A:368:LEU:N	1:A:369:PRO:HD3	1.91	0.86
1:C:39:ILE:HG21	1:C:205:LEU:HD21	1.60	0.83
1:A:367:LYS:C	1:A:368:LEU:CD2	2.42	0.82
1:C:448:ASN:C	1:C:448:ASN:ND2	2.30	0.80
1:B:105:LEU:HD13	1:B:359:LEU:HD21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD23	1:A:368:LEU:N	1.86	0.79
1:C:448:ASN:ND2	1:C:449:PRO:N	2.30	0.79
1:A:371:LEU:HD23	1:A:371:LEU:C	2.00	0.78
1:A:368:LEU:N	1:A:369:PRO:CD	2.45	0.78
1:A:367:LYS:C	1:A:369:PRO:HD3	2.03	0.78
1:A:371:LEU:O	1:A:371:LEU:CD2	2.30	0.77
1:A:373:GLY:O	1:A:375:GLU:N	2.18	0.77
1:A:167:THR:O	1:A:167:THR:HG22	1.87	0.75
1:A:440:LEU:HD13	1:A:443:LEU:HD23	1.69	0.74
1:C:219:ASN:HB3	1:C:232:LEU:HD23	1.70	0.73
1:C:448:ASN:HD22	1:C:449:PRO:N	1.87	0.72
1:A:169:LEU:HD11	1:A:303:LEU:HB3	1.73	0.71
1:A:449:PRO:O	1:A:450:GLN:C	2.29	0.70
1:A:105:LEU:HD22	1:A:359:LEU:HD11	1.74	0.70
1:C:237:VAL:HG11	1:C:244:LEU:HD21	1.72	0.69
1:C:39:ILE:CG2	1:C:205:LEU:HD21	2.22	0.69
1:B:3:VAL:HG22	1:B:3:VAL:O	1.91	0.68
1:A:105:LEU:CD2	1:A:359:LEU:HD11	2.22	0.68
1:A:193:LEU:HD23	1:A:200:LEU:HD11	1.76	0.68
1:A:371:LEU:C	1:A:371:LEU:CD2	2.62	0.67
1:A:33:THR:HG21	1:A:383:ASP:HB3	1.78	0.66
1:B:336:ILE:HG23	1:B:336:ILE:O	1.96	0.66
1:A:367:LYS:C	1:A:369:PRO:CD	2.65	0.64
1:A:448:ASN:OD1	1:A:449:PRO:N	2.30	0.64
1:C:348:LEU:HB3	1:C:424:LEU:HD12	1.77	0.64
1:C:448:ASN:ND2	1:C:449:PRO:O	2.30	0.64
1:B:449:PRO:O	1:B:450:GLN:C	2.30	0.64
1:D:51:LEU:HD21	1:D:199:ALA:HB2	1.80	0.64
1:A:448:ASN:OD1	1:A:448:ASN:C	2.33	0.63
1:C:12:TYR:OH	1:C:130:VAL:HG13	1.98	0.63
1:A:344:ILE:HD13	1:A:420:LEU:HB3	1.81	0.63
1:D:127:LEU:HD21	1:D:363:LEU:HD21	1.82	0.62
1:D:333:LEU:CD1	1:D:440:LEU:HD11	2.26	0.62
1:C:392:LEU:HD23	1:C:393:ASN:N	2.14	0.62
1:A:150:LEU:O	1:A:153:VAL:HG22	2.00	0.62
1:A:368:LEU:N	1:A:368:LEU:CD2	2.48	0.61
1:C:100:LEU:C	1:C:100:LEU:HD23	2.21	0.61
1:A:55:LEU:HD22	1:A:155:GLY:HA2	1.83	0.60
1:C:108:THR:HG23	1:C:245:PHE:CE2	2.37	0.60
1:D:225:VAL:HG23	1:D:226:THR:HG23	1.84	0.60
1:D:254:THR:HG23	1:D:402:GLY:HA2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:SER:C	1:A:273:ILE:HD12	2.22	0.59
1:B:193:LEU:HD23	1:B:200:LEU:HD11	1.83	0.59
1:A:254:THR:HG23	1:A:402:GLY:HA2	1.85	0.58
1:C:314:PRO:HG3	1:C:320:LEU:HD13	1.86	0.58
1:C:348:LEU:CB	1:C:424:LEU:HD12	2.35	0.57
1:D:175:VAL:HG23	1:D:197:THR:HG21	1.87	0.57
1:D:157:LEU:HD13	1:D:441:HIS:CD2	2.39	0.56
1:C:39:ILE:HG21	1:C:205:LEU:CD2	2.33	0.56
1:C:286:PHE:CG	1:C:301:VAL:HG12	2.40	0.56
1:B:12:TYR:OH	1:B:130:VAL:HG13	2.06	0.56
1:C:259:SER:HA	1:C:401:ALA:HB1	1.87	0.56
1:D:169:LEU:HD11	1:D:303:LEU:HB3	1.88	0.56
1:C:272:SER:OG	1:C:273:ILE:HD12	2.07	0.55
1:C:286:PHE:CD2	1:C:301:VAL:HG12	2.42	0.54
1:A:317:ILE:HD12	1:A:317:ILE:H	1.73	0.53
1:B:225:VAL:HG23	1:B:226:THR:HG23	1.89	0.53
1:B:319:ASP:O	1:B:323:VAL:HG23	2.08	0.53
1:B:3:VAL:O	1:B:3:VAL:CG2	2.56	0.53
1:C:39:ILE:CG2	1:C:205:LEU:CD2	2.86	0.53
1:C:219:ASN:CB	1:C:232:LEU:HD23	2.38	0.53
1:B:344:ILE:CD1	1:B:420:LEU:HD23	2.38	0.53
1:C:47:ASN:O	1:C:51:LEU:HD13	2.09	0.53
1:D:207:LEU:HD12	1:D:241:SER:O	2.09	0.52
1:D:344:ILE:HD13	1:D:420:LEU:HB3	1.91	0.52
1:A:62:LEU:HD22	1:A:66:ASP:HB3	1.91	0.52
1:C:100:LEU:HD23	1:C:101:SER:N	2.24	0.52
1:C:254:THR:HG23	1:C:402:GLY:HA2	1.91	0.52
1:D:55:LEU:HD22	1:D:155:GLY:HA2	1.92	0.52
1:A:55:LEU:HD22	1:A:155:GLY:CA	2.39	0.52
1:A:56:VAL:HG13	1:A:159:THR:HG21	1.91	0.52
1:C:106:PHE:CE2	1:C:128:LEU:HD13	2.45	0.51
1:D:150:LEU:O	1:D:153:VAL:HG22	2.10	0.51
1:A:353:ILE:HD11	1:A:446:VAL:HG22	1.93	0.51
1:B:190:VAL:HG11	1:C:29:LEU:CD1	2.41	0.51
1:C:324:GLU:HA	1:C:429:LEU:HD11	1.93	0.51
1:C:448:ASN:ND2	1:C:449:PRO:C	2.64	0.51
1:C:1:ASP:OD1	1:C:1:ASP:N	2.42	0.51
1:D:333:LEU:HD22	1:D:335:TRP:CZ2	2.46	0.50
1:C:317:ILE:HD12	1:C:317:ILE:H	1.77	0.50
1:C:175:VAL:HB	1:C:200:LEU:HD12	1.93	0.50
1:D:286:PHE:CG	1:D:301:VAL:HG12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:PRO:O	1:B:450:GLN:O	2.30	0.50
1:C:62:LEU:HD22	1:C:66:ASP:HB3	1.94	0.50
1:B:344:ILE:HD13	1:B:420:LEU:HB3	1.94	0.49
1:A:70:ALA:O	1:A:73:VAL:HG12	2.12	0.49
1:A:449:PRO:O	1:A:450:GLN:O	2.29	0.49
1:B:105:LEU:HD22	1:B:359:LEU:HD11	1.94	0.49
1:A:420:LEU:CD1	1:B:420:LEU:HD13	2.43	0.49
1:A:125:GLN:HE22	1:A:140:ARG:HD3	1.76	0.49
1:C:449:PRO:O	1:C:450:GLN:O	2.30	0.49
1:A:286:PHE:CG	1:A:301:VAL:HG12	2.48	0.49
1:A:420:LEU:HD11	1:B:420:LEU:HD13	1.93	0.49
1:B:51:LEU:HD21	1:B:199:ALA:HB2	1.93	0.49
1:B:101:SER:HB3	1:B:104:ALA:HB3	1.95	0.49
1:B:169:LEU:HD23	1:B:251:PHE:CE1	2.47	0.49
1:B:219:ASN:HB3	1:B:232:LEU:HD12	1.94	0.49
1:B:174:VAL:HG22	1:B:248:TYR:HB2	1.95	0.49
1:D:77:THR:O	1:D:80:VAL:HG12	2.13	0.49
1:A:243:LEU:O	1:A:244:LEU:HD23	2.13	0.48
1:B:230:MET:O	1:B:232:LEU:HD22	2.12	0.48
1:A:373:GLY:O	1:A:374:ALA:C	2.50	0.48
1:B:169:LEU:HD11	1:B:303:LEU:HB3	1.95	0.48
1:B:244:LEU:HD22	1:B:390:GLU:HG2	1.96	0.48
1:A:51:LEU:HD21	1:A:199:ALA:HB2	1.94	0.48
1:B:156:LEU:O	1:B:159:THR:HG22	2.14	0.48
1:D:397:LEU:HD23	1:D:398:GLU:N	2.29	0.48
1:B:142:ASP:O	1:B:146:VAL:HG23	2.13	0.48
1:B:221:PHE:O	1:B:225:VAL:HG22	2.14	0.47
1:B:237:VAL:HG11	1:B:244:LEU:HD21	1.95	0.47
1:D:320:LEU:HD21	1:D:445:ARG:HD2	1.96	0.47
1:C:106:PHE:HE2	1:C:128:LEU:HD13	1.80	0.47
1:C:323:VAL:O	1:C:327:ILE:HG22	2.14	0.47
1:D:117:LEU:HD21	1:D:380:ASN:HD21	1.79	0.47
1:D:59:ALA:HB2	1:D:155:GLY:HA3	1.96	0.47
1:B:197:THR:HG23	1:B:197:THR:O	2.15	0.47
1:C:313:GLN:HG3	1:C:424:LEU:HD23	1.97	0.47
1:C:336:ILE:O	1:C:336:ILE:HG22	2.14	0.47
1:A:52:HIS:O	1:A:56:VAL:HG23	2.15	0.46
1:B:329:GLN:O	1:B:331:ASP:N	2.48	0.46
1:C:149:ALA:O	1:C:153:VAL:HG13	2.15	0.46
1:B:127:LEU:HD21	1:B:363:LEU:HD21	1.98	0.46
1:A:169:LEU:HD21	1:A:307:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD13	1:B:196:PHE:HB2	1.97	0.46
1:B:357:TYR:O	1:B:392:LEU:HD12	2.14	0.46
1:C:255:MET:HE3	1:C:258:PHE:CZ	2.50	0.46
1:B:243:LEU:HD13	1:B:244:LEU:N	2.30	0.46
1:D:424:LEU:HD23	1:D:428:PHE:CG	2.51	0.46
1:B:88:LEU:HA	1:B:362:LEU:HD22	1.97	0.46
1:C:243:LEU:HD23	1:C:244:LEU:N	2.31	0.46
1:D:392:LEU:HD23	1:D:393:ASN:N	2.31	0.46
1:D:397:LEU:HD23	1:D:397:LEU:C	2.36	0.46
1:A:373:GLY:C	1:A:375:GLU:N	2.68	0.45
1:A:353:ILE:HD11	1:A:446:VAL:CG2	2.46	0.45
1:D:125:GLN:HG3	1:D:141:LEU:HD12	1.99	0.45
1:D:317:ILE:HD12	1:D:317:ILE:H	1.80	0.45
1:B:79:PHE:CE1	1:B:129:ASP:HB2	2.51	0.45
1:B:272:SER:HB2	1:B:273:ILE:HG23	1.98	0.45
1:D:279:MET:CE	1:D:347:THR:HG22	2.47	0.45
1:A:397:LEU:HD23	1:A:398:GLU:N	2.32	0.45
1:B:106:PHE:CE2	1:B:128:LEU:HD13	2.52	0.45
1:C:105:LEU:CD2	1:C:359:LEU:HD11	2.46	0.45
1:A:167:THR:O	1:A:167:THR:CG2	2.59	0.45
1:D:79:PHE:CE1	1:D:129:ASP:HB2	2.52	0.45
1:C:329:GLN:O	1:C:331:ASP:N	2.50	0.44
1:D:243:LEU:HD22	1:D:244:LEU:N	2.32	0.44
1:A:189:PHE:CZ	1:A:193:LEU:HD11	2.52	0.44
1:A:243:LEU:HD22	1:A:244:LEU:N	2.33	0.44
1:B:317:ILE:HD12	1:B:317:ILE:H	1.83	0.44
1:C:292:ALA:HB1	1:D:425:SER:OG	2.18	0.44
1:B:450:GLN:OE1	1:B:450:GLN:HA	2.17	0.44
1:D:174:VAL:HG12	1:D:199:ALA:HB1	2.00	0.44
1:A:105:LEU:HD22	1:A:359:LEU:HD21	1.99	0.44
1:C:106:PHE:O	1:C:110:VAL:HG23	2.17	0.44
1:D:273:ILE:HD12	1:D:273:ILE:N	2.33	0.44
1:C:124:LEU:HG	1:C:371:LEU:HD21	2.00	0.43
1:A:77:THR:HG22	1:A:102:PRO:HB2	1.99	0.43
1:C:332:LEU:HB3	1:C:334:THR:HG23	1.99	0.43
1:A:440:LEU:CD1	1:A:443:LEU:HD23	2.45	0.43
1:B:268:TRP:HZ3	1:B:317:ILE:HG21	1.83	0.43
1:A:59:ALA:HB2	1:A:155:GLY:HA3	1.99	0.43
1:D:34:PHE:HA	1:D:184:ARG:NH2	2.34	0.43
1:A:175:VAL:HG23	1:A:197:THR:HG21	2.01	0.43
1:A:329:GLN:O	1:A:331:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:SER:HB2	1:B:347:THR:HG23	2.01	0.43
1:C:175:VAL:HG23	1:C:197:THR:HG21	2.01	0.43
1:C:244:LEU:HD22	1:C:390:GLU:HG2	2.00	0.43
1:D:52:HIS:CD2	1:D:170:LEU:HD23	2.53	0.43
1:D:303:LEU:HD11	1:D:309:LEU:HB2	2.00	0.43
1:A:343:ALA:HB1	1:A:419:ALA:HB2	1.99	0.43
1:B:8:PHE:HB3	1:B:11:LEU:HD12	2.01	0.43
1:D:329:GLN:O	1:D:331:ASP:N	2.52	0.43
1:D:392:LEU:C	1:D:393:ASN:HD22	2.22	0.43
1:B:105:LEU:CD1	1:B:359:LEU:HD21	2.42	0.43
1:C:370:THR:HG21	1:C:375:GLU:OE1	2.19	0.43
1:C:48:GLU:OE2	1:C:250:HIS:ND1	2.41	0.43
1:C:51:LEU:HD21	1:C:199:ALA:HB2	1.99	0.43
1:C:181:PRO:HD3	1:C:205:LEU:O	2.19	0.42
1:C:169:LEU:HD11	1:C:303:LEU:HB3	2.01	0.42
1:C:340:PRO:HA	1:C:341:PRO:HD3	1.92	0.42
1:A:373:GLY:C	1:A:375:GLU:H	2.22	0.42
1:C:156:LEU:HD22	1:C:306:ARG:NH2	2.34	0.42
1:D:180:ALA:HB2	1:D:242:THR:HA	2.00	0.42
1:D:215:THR:HG21	1:D:233:PRO:O	2.20	0.42
1:D:174:VAL:HG12	1:D:199:ALA:CB	2.50	0.42
1:D:344:ILE:HG23	1:D:422:VAL:HG23	2.00	0.42
1:A:77:THR:O	1:A:80:VAL:HG12	2.20	0.42
1:B:424:LEU:HD23	1:B:428:PHE:CD1	2.54	0.42
1:D:323:VAL:O	1:D:327:ILE:HG22	2.20	0.42
1:A:11:LEU:CD1	1:A:76:ILE:HD11	2.50	0.42
1:A:114:LEU:HD13	1:A:192:SER:HB3	2.01	0.42
1:B:336:ILE:O	1:B:336:ILE:CG2	2.66	0.42
1:D:332:LEU:HB3	1:D:334:THR:HG23	2.01	0.42
1:A:8:PHE:HB3	1:A:11:LEU:HD12	2.02	0.41
1:B:159:THR:O	1:B:159:THR:HG23	2.20	0.41
1:B:174:VAL:HG13	1:B:228:TRP:CH2	2.55	0.41
1:B:175:VAL:HG23	1:B:197:THR:HG21	2.01	0.41
1:C:268:TRP:O	1:C:427:PRO:HD3	2.21	0.41
1:A:312:ILE:N	1:A:312:ILE:HD12	2.35	0.41
1:B:392:LEU:C	1:B:393:ASN:HD22	2.23	0.41
1:C:118:ASP:OD2	1:C:140:ARG:NH1	2.49	0.41
1:C:150:LEU:O	1:C:153:VAL:HG22	2.20	0.41
1:C:392:LEU:HD23	1:C:393:ASN:C	2.40	0.41
1:C:397:LEU:HD23	1:C:398:GLU:N	2.35	0.41
1:D:254:THR:HG23	1:D:402:GLY:CA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ILE:HG22	1:B:396:LEU:N	2.36	0.41
1:C:33:THR:HG22	1:C:186:LYS:HA	2.03	0.41
1:C:295:ASN:ND2	1:D:317:ILE:HD11	2.36	0.41
1:D:156:LEU:HD22	1:D:306:ARG:CZ	2.50	0.41
1:B:351:LEU:HD12	1:B:399:LEU:HD22	2.02	0.40
1:B:267:PHE:HE2	1:B:447:ASN:O	2.04	0.40
1:B:301:VAL:HA	1:B:302:PRO:HD3	1.95	0.40
1:B:33:THR:HG22	1:B:186:LYS:HA	2.02	0.40
1:C:232:LEU:HD12	1:C:232:LEU:HA	1.92	0.40
1:A:178:PHE:CE2	1:A:218:ILE:HG23	2.56	0.40
1:A:243:LEU:HD12	1:A:388:VAL:HG22	2.04	0.40
1:D:392:LEU:HD23	1:D:393:ASN:C	2.42	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	403/453 (89%)	383 (95%)	17 (4%)	3 (1%)	22	56
1	B	422/453 (93%)	402 (95%)	17 (4%)	3 (1%)	22	56
1	C	415/453 (92%)	393 (95%)	22 (5%)	0	100	100
1	D	403/453 (89%)	385 (96%)	18 (4%)	0	100	100
All	All	1643/1812 (91%)	1563 (95%)	74 (4%)	6 (0%)	34	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ALA
1	B	449	PRO
1	B	199	ALA

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Mol	Chain	Res	Type
1	B	336	ILE
1	A	449	PRO
1	A	336	ILE

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	354/394 (90%)	334 (94%)	20 (6%)	21	53
1	B	371/394 (94%)	356 (96%)	15 (4%)	31	64
1	C	364/394 (92%)	342 (94%)	22 (6%)	19	50
1	D	352/394 (89%)	339 (96%)	13 (4%)	34	66
All	All	1441/1576 (91%)	1371 (95%)	70 (5%)	25	58

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	42	LYS
1	A	55	LEU
1	A	63	GLU
1	A	83	ARG
1	A	105	LEU
1	A	174	VAL
1	A	231	ASN
1	A	232	LEU
1	A	237	VAL
1	A	239	THR
1	A	271	ASN
1	A	315	HIS
1	A	316	CYS
1	A	365	GLU
1	A	368	LEU
1	A	370	THR
1	A	394	SER

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Mol	Chain	Res	Type
1	A	434	GLU
1	A	450	GLN
1	B	1	ASP
1	B	3	VAL
1	B	10	LEU
1	B	17	THR
1	B	44	SER
1	B	63	GLU
1	B	105	LEU
1	B	174	VAL
1	B	223	LYS
1	B	269	VAL
1	B	272	SER
1	B	293	GLN
1	B	316	CYS
1	B	434	GLU
1	B	436	ASP
1	C	1	ASP
1	C	17	THR
1	C	80	VAL
1	C	96	SER
1	C	105	LEU
1	C	111	SER
1	C	120	THR
1	C	153	VAL
1	C	154	GLN
1	C	174	VAL
1	C	232	LEU
1	C	237	VAL
1	C	243	LEU
1	C	315	HIS
1	C	316	CYS
1	C	341	PRO
1	C	342	ARG
1	C	370	THR
1	C	393	ASN
1	C	434	GLU
1	C	443	LEU
1	C	448	ASN
1	D	55	LEU
1	D	63	GLU
1	D	105	LEU

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Mol	Chain	Res	Type
1	D	159	THR
1	D	205	LEU
1	D	232	LEU
1	D	243	LEU
1	D	315	HIS
1	D	352	GLU
1	D	360	GLN
1	D	393	ASN
1	D	434	GLU
1	D	436	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	271	ASN
1	B	295	ASN
1	B	393	ASN
1	B	447	ASN
1	C	9	HIS
1	C	350	GLN
1	C	448	ASN
1	D	380	ASN
1	D	393	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 (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(Å^2)	Q<0.9
1	A	412/453 (90%)	0.28	11 (2%)	54	38	50, 76, 114, 130	9 (2%)
1	B	428/453 (94%)	0.33	20 (4%)	31	20	46, 77, 113, 142	9 (2%)
1	C	422/453 (93%)	0.29	13 (3%)	49	32	26, 88, 118, 138	9 (2%)
1	D	411/453 (90%)	0.65	49 (11%)	4	2	52, 118, 182, 230	9 (2%)
All	All	1673/1812 (92%)	0.38	93 (5%)	24	15	26, 87, 148, 230	36 (2%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	GLY	6.5
1	D	335	TRP	6.3
1	D	440	LEU	5.1
1	D	336	ILE	4.4
1	D	337	GLU	4.4
1	D	419	ALA	3.9
1	C	134	GLU	3.8
1	D	289	TRP	3.8
1	D	326	LEU	3.7
1	D	296	PHE	3.6
1	D	236	GLY	3.5
1	D	260	GLN	3.5
1	D	432	ILE	3.5
1	D	334	THR	3.4
1	D	292	ALA	3.3
1	D	211	PRO	3.3
1	D	310	LEU	3.3
1	D	299	THR	3.2
1	B	433	TYR	3.2
1	C	367	LYS	3.2
1	D	363	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	313	GLN	3.1
1	B	264	VAL	3.1
1	D	332	LEU	3.1
1	C	359	LEU	3.0
1	D	207	LEU	2.9
1	B	424	LEU	2.9
1	A	335	TRP	2.9
1	D	367	LYS	2.9
1	A	440	LEU	2.8
1	B	431	ALA	2.8
1	C	365	GLU	2.8
1	D	293	GLN	2.8
1	D	353	ILE	2.8
1	D	286	PHE	2.8
1	B	353	ILE	2.8
1	D	327	ILE	2.8
1	B	317	ILE	2.7
1	B	430	PHE	2.7
1	D	328	PHE	2.7
1	D	182	GLY	2.7
1	C	4	TYR	2.6
1	B	443	LEU	2.6
1	D	369	PRO	2.6
1	B	331	ASP	2.6
1	C	267	PHE	2.6
1	D	297	SER	2.6
1	A	422	VAL	2.5
1	B	313	GLN	2.5
1	D	378	LEU	2.5
1	D	272	SER	2.5
1	D	219	ASN	2.5
1	D	359	LEU	2.5
1	D	420	LEU	2.5
1	C	424	LEU	2.5
1	A	99	ILE	2.4
1	D	340	PRO	2.4
1	B	365	GLU	2.4
1	D	287	GLN	2.4
1	A	98	ALA	2.4
1	C	311	LEU	2.4
1	C	289	TRP	2.3
1	C	39	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	89	ASN	2.3
1	D	303	LEU	2.3
1	B	59	ALA	2.3
1	B	346	LEU	2.3
1	B	442	PHE	2.3
1	B	343	ALA	2.3
1	A	365	GLU	2.2
1	B	440	LEU	2.2
1	C	124	LEU	2.2
1	D	443	LEU	2.2
1	D	341	PRO	2.2
1	B	4	TYR	2.2
1	D	275	VAL	2.2
1	D	298	VAL	2.2
1	A	196	PHE	2.1
1	D	399	LEU	2.1
1	B	310	LEU	2.1
1	A	424	LEU	2.1
1	C	303	LEU	2.1
1	D	132	VAL	2.1
1	D	315	HIS	2.1
1	A	443	LEU	2.1
1	A	366	ASP	2.1
1	D	48	GLU	2.1
1	B	429	LEU	2.0
1	D	90	GLU	2.0
1	D	80	VAL	2.0
1	D	100	LEU	2.0
1	A	61	LYS	2.0
1	D	61	LYS	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.