Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 01:59 pm BST

PDB ID	:	1KHU
Title	:	Smad1 crystal structure reveals the details of BMP signaling pathway
Authors	:	Qin, B.Y.; Lin, K.
Deposited on	:	2001-12-01
Resolution	:	2.50 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 following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.50 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	Percentile Ranks	Value
Rfree		0.271
Clashscore		30
Ramachandran outliers		2.0%
Sidechain outliers		7.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
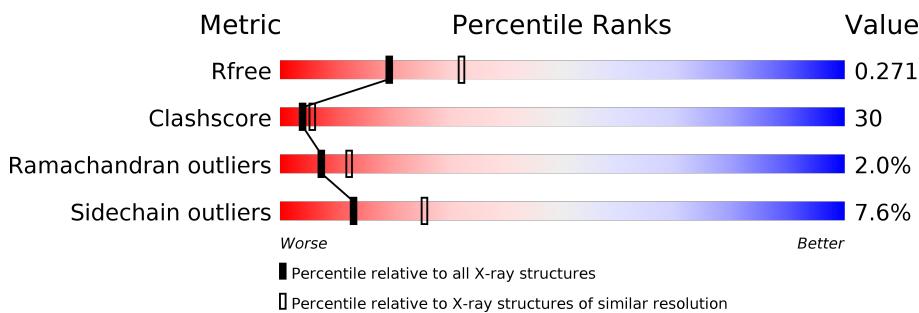
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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%

Mol	Chain	Length	Quality of chain
1	A	218	50% 36% 5% 9%
1	B	218	45% 39% 6% 10%
1	C	218	50% 35% 6% 10%
1	D	218	48% 32% • 16%
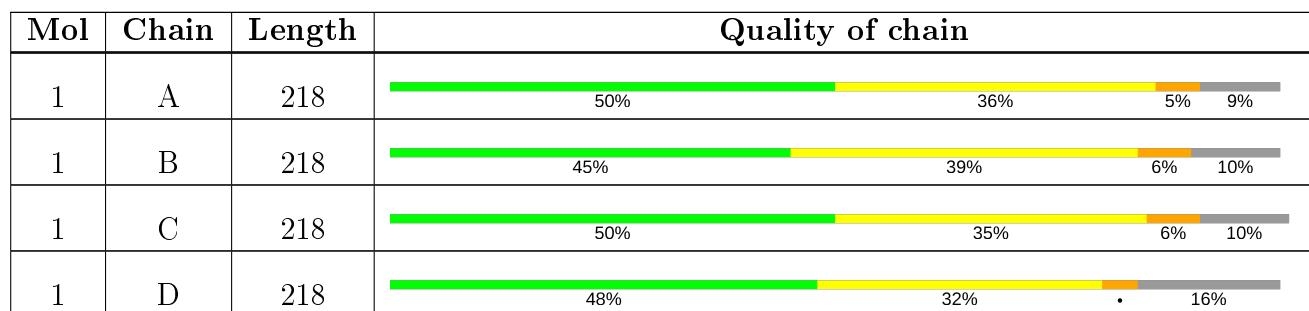
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6772 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 SMAD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1575	993	280	291	11			
1	B	197	Total	C	N	O	S	0	0	0
			1568	988	279	290	11			
1	C	197	Total	C	N	O	S	0	0	0
			1568	988	279	290	11			
1	D	184	Total	C	N	O	S	0	0	0
			1475	932	262	271	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	135	Total	O	0	0
			135	135		
2	C	150	Total	O	0	0
			150	150		
2	D	153	Total	O	0	0
			153	153		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: SMAD1

Chain A:

- Molecule 1: SMAD1
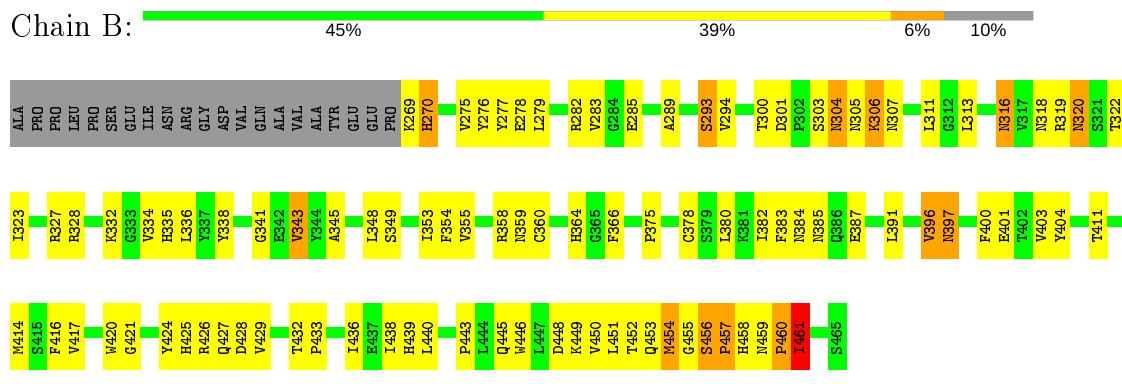
Chain B:

- Molecule 1: SMAD1
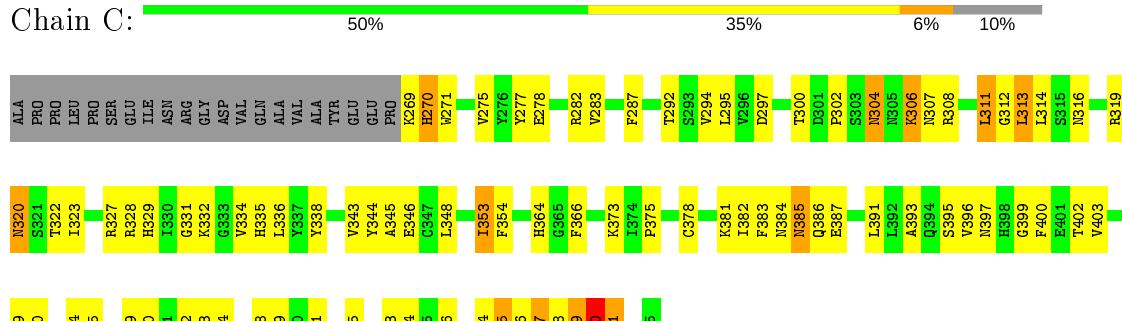
Chain C:

• Molecule 1: SMAD1

Chain D:

48%   32%   •   16%
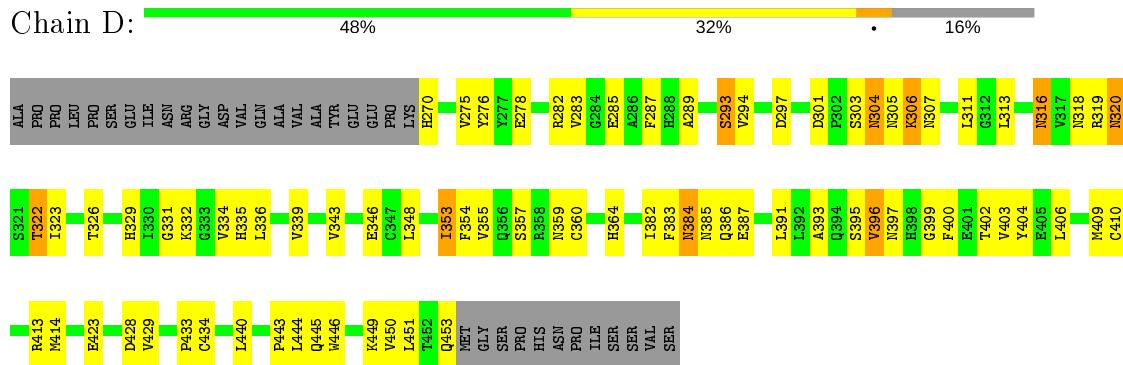
4   Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	138.13Å 138.13Å 199.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.00 – 2.50 38.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.00-2.50) 93.6 (38.29-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.19 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.274 0.240 , 0.271	Depositor DCC
R_{free} test set	2380 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.9	EDS
L-test for twinning[2]	$<|L|> = 0.39, <L^2> = 0.21$	Xtriage
Estimated twinning fraction	0.329 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6772	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 0.333 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	0.41	0/1619	0.66	0/2197
1	B	0.41	0/1611	0.65	1/2186 (0.0%)
1	C	0.40	0/1611	0.66	1/2186 (0.0%)
1	D	0.45	0/1515	0.68	0/2057
All	All	0.42	0/6356	0.67	2/8626 (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	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	300	THR	N-CA-C	5.43	125.67	111.00
1	C	300	THR	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	277	TYR	Sidechain

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	1575	0	1509	100	0
1	B	1568	0	1501	104	0
1	C	1568	0	1501	98	0
1	D	1475	0	1409	82	0
2	A	148	0	0	15	0
2	B	135	0	0	10	0
2	C	150	0	0	23	0
2	D	153	0	0	18	0
All	All	6772	0	5920	367	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 30.

All (367) 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:C:384:ASN:ND2	1:C:387:GLU:HG3	1.76	1.00
1:A:359:ASN:HD22	1:A:383:PHE:HA	1.30	0.93
1:B:396:VAL:HG13	1:B:397:ASN:H	1.34	0.92
1:A:328:ARG:HG2	1:B:404:TYR:HE1	1.34	0.90
1:D:282:ARG:HH21	1:D:282:ARG:HG2	1.39	0.88
1:A:328:ARG:HG2	1:B:404:TYR:CE1	2.11	0.86
1:D:294:VAL:HG22	1:D:336:LEU:HB2	1.58	0.84
1:A:359:ASN:ND2	1:A:383:PHE:HA	1.95	0.82
1:B:294:VAL:HG22	1:B:336:LEU:HB2	1.59	0.82
1:C:343:VAL:HG22	1:C:383:PHE:HB3	1.61	0.81
1:C:373:LYS:HD2	2:C:564:HOH:O	1.80	0.81
1:D:396:VAL:HG13	1:D:397:ASN:H	1.44	0.81
1:B:458:HIS:HB2	2:B:520:HOH:O	1.81	0.81
1:A:451:LEU:HD12	2:C:473:HOH:O	1.82	0.80
1:A:385:ASN:HD22	1:A:446:TRP:HH2	1.30	0.79
1:A:359:ASN:HD21	1:A:384:ASN:H	1.30	0.79
1:D:413:ARG:HD3	2:D:542:HOH:O	1.83	0.79
1:A:456:SER:HB2	2:A:613:HOH:O	1.84	0.78
1:A:455:GLY:O	1:A:457:PRO:HD3	1.84	0.78
1:A:275:VAL:HG22	1:A:282:ARG:NH1	2.00	0.77
1:C:313:LEU:HD13	2:C:500:HOH:O	1.85	0.77
1:C:384:ASN:HD22	1:C:387:GLU:H	1.33	0.76
1:A:320:ASN:HD22	1:A:320:ASN:C	1.88	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:CG2	1:B:336:LEU:HB2	2.15	0.75
1:A:447:LEU:HG	2:C:473:HOH:O	1.87	0.75
1:A:268:PRO:HB2	1:A:290:SER:O	1.86	0.75
1:D:429:VAL:HG21	2:D:542:HOH:O	1.86	0.74
1:C:461:ILE:H	1:C:461:ILE:HD13	1.52	0.74
1:D:278:GLU:HG3	1:D:283:VAL:HG21	1.66	0.74
1:D:384:ASN:HD22	1:D:387:GLU:H	1.36	0.74
1:C:393:ALA:O	1:C:396:VAL:HG12	1.87	0.74
1:B:278:GLU:HG3	1:B:283:VAL:HG21	1.69	0.73
1:B:332:LYS:HZ2	1:C:459:ASN:N	1.87	0.73
1:D:294:VAL:CG2	1:D:336:LEU:HB2	2.18	0.73
1:B:316:ASN:ND2	1:B:318:ASN:H	1.87	0.72
1:B:282:ARG:HG2	1:B:282:ARG:HH21	1.55	0.72
1:A:368:PRO:HB2	2:A:511:HOH:O	1.89	0.72
1:B:338:TYR:HD2	1:B:343:VAL:HG12	1.55	0.71
1:C:345:ALA:HB1	2:C:505:HOH:O	1.91	0.71
1:B:278:GLU:HA	1:B:433:PRO:O	1.90	0.71
1:B:332:LYS:NZ	1:C:458:HIS:HA	2.07	0.70
1:B:320:ASN:HD21	1:B:323:ILE:HG13	1.55	0.70
1:A:404:TYR:HE1	1:C:328:ARG:HG2	1.57	0.70
1:C:282:ARG:HG2	1:C:282:ARG:HH21	1.57	0.69
1:C:384:ASN:ND2	1:C:387:GLU:H	1.89	0.69
1:A:452:THR:HG21	2:A:525:HOH:O	1.91	0.69
1:A:384:ASN:ND2	1:A:387:GLU:H	1.89	0.69
1:D:434:CYS:SG	2:D:585:HOH:O	2.50	0.69
1:D:384:ASN:HD21	1:D:386:GLN:HB3	1.57	0.69
1:A:359:ASN:ND2	1:A:384:ASN:H	1.89	0.69
1:A:320:ASN:ND2	1:A:322:THR:HG23	2.08	0.68
1:C:332:LYS:HG2	2:C:520:HOH:O	1.93	0.68
1:B:332:LYS:HE3	1:C:457:PRO:HG2	1.75	0.68
1:D:282:ARG:NH2	1:D:282:ARG:HG2	2.08	0.68
1:B:396:VAL:HG13	1:B:397:ASN:N	2.08	0.68
1:C:334:VAL:HB	1:C:353:ILE:HD13	1.75	0.68
1:D:396:VAL:HG13	1:D:397:ASN:N	2.08	0.68
1:B:359:ASN:ND2	1:B:384:ASN:H	1.92	0.68
1:C:275:VAL:HG22	1:C:282:ARG:NH1	2.08	0.68
1:A:450:VAL:O	1:A:453:GLN:HG2	1.93	0.67
1:B:332:LYS:HZ1	1:C:458:HIS:HA	1.59	0.67
1:C:384:ASN:HD21	1:C:386:GLN:HB3	1.59	0.67
1:B:349:SER:HA	2:B:471:HOH:O	1.92	0.67
1:B:461:ILE:N	1:B:461:ILE:HD12	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ASN:C	1:C:320:ASN:HD22	1.97	0.67
1:C:278:GLU:HG3	1:C:283:VAL:HG21	1.75	0.67
1:C:461:ILE:N	1:C:461:ILE:HD13	2.10	0.67
1:D:285:GLU:HG3	2:D:496:HOH:O	1.93	0.67
1:C:343:VAL:HG22	1:C:383:PHE:CB	2.25	0.66
1:A:335:HIS:HB3	1:A:346:GLU:HB3	1.78	0.66
1:A:400:PHE:CE2	1:A:454:MET:HB3	2.29	0.65
1:C:313:LEU:HD22	2:C:500:HOH:O	1.94	0.65
1:A:268:PRO:CA	1:A:291:SER:HA	2.27	0.65
1:D:429:VAL:HG11	2:D:542:HOH:O	1.97	0.65
1:D:334:VAL:HB	1:D:353:ILE:HD13	1.77	0.65
1:A:316:ASN:ND2	1:A:318:ASN:H	1.94	0.64
1:C:410:CYS:HB3	1:C:444:LEU:HG	1.78	0.64
1:D:384:ASN:ND2	1:D:387:GLU:H	1.96	0.64
1:B:452:THR:HA	1:B:454:MET:HE2	1.80	0.64
1:D:343:VAL:HG23	1:D:382:ILE:HG12	1.80	0.63
1:B:359:ASN:HD21	1:B:384:ASN:H	1.45	0.63
1:B:403:VAL:HG11	1:B:453:GLN:HE22	1.62	0.63
1:D:320:ASN:C	1:D:320:ASN:HD22	2.02	0.63
1:D:359:ASN:ND2	1:D:384:ASN:H	1.97	0.63
1:D:332:LYS:HE2	2:D:467:HOH:O	1.98	0.63
1:A:407:THR:HG22	2:C:614:HOH:O	1.98	0.63
1:B:455:GLY:C	1:B:457:PRO:HD3	2.19	0.62
1:A:275:VAL:HG22	1:A:282:ARG:HH11	1.63	0.62
1:B:320:ASN:ND2	1:B:323:ILE:H	1.96	0.62
1:C:384:ASN:HD22	1:C:387:GLU:HG3	1.62	0.62
1:A:404:TYR:CE1	1:C:328:ARG:HG2	2.34	0.62
1:C:278:GLU:OE2	1:C:327:ARG:HD2	2.00	0.61
1:A:384:ASN:HD22	1:A:387:GLU:H	1.48	0.61
1:D:343:VAL:HG23	1:D:382:ILE:CG1	2.31	0.60
1:D:413:ARG:HB3	2:D:542:HOH:O	2.01	0.60
1:B:425:HIS:O	1:B:426:ARG:HB2	2.00	0.60
1:A:400:PHE:HA	1:A:403:VAL:HG12	1.84	0.60
1:A:268:PRO:HA	1:A:291:SER:HA	1.84	0.59
1:D:326:THR:HB	2:D:585:HOH:O	2.01	0.59
1:D:343:VAL:HG22	1:D:383:PHE:HB3	1.84	0.59
1:B:375:PRO:HB2	1:B:378:CYS:SG	2.42	0.59
1:A:268:PRO:CB	1:A:291:SER:HA	2.31	0.59
1:B:332:LYS:HZ2	1:C:459:ASN:H	1.51	0.59
1:C:343:VAL:HG23	1:C:382:ILE:HG13	1.85	0.59
1:C:320:ASN:ND2	1:C:323:ILE:H	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:VAL:HB	1:B:353:ILE:HD13	1.84	0.58
1:C:399:GLY:HA3	2:C:524:HOH:O	2.02	0.58
1:A:404:TYR:HE2	2:C:586:HOH:O	1.87	0.58
1:A:322:THR:HG22	2:A:590:HOH:O	2.04	0.58
1:B:432:THR:HB	2:B:483:HOH:O	2.04	0.58
1:B:396:VAL:HG22	1:B:397:ASN:N	2.19	0.58
1:B:450:VAL:O	1:B:453:GLN:HB3	2.03	0.58
1:C:334:VAL:HB	1:C:353:ILE:CD1	2.33	0.57
1:A:400:PHE:HE2	1:A:454:MET:HB3	1.69	0.57
1:C:282:ARG:HG2	1:C:282:ARG:NH2	2.17	0.57
1:C:332:LYS:HD2	2:C:542:HOH:O	2.04	0.57
1:D:359:ASN:HD21	1:D:384:ASN:H	1.50	0.57
1:B:334:VAL:HB	1:B:353:ILE:CD1	2.35	0.57
1:A:367:HIS:HB2	2:A:523:HOH:O	2.05	0.57
1:B:425:HIS:HB2	1:B:427:GLN:HG2	1.87	0.57
1:B:279:LEU:CD1	1:B:323:ILE:HD11	2.35	0.56
1:D:316:ASN:ND2	1:D:318:ASN:H	2.04	0.56
1:A:285:GLU:HG3	2:A:531:HOH:O	2.05	0.56
1:B:269:LYS:NZ	1:B:269:LYS:HB2	2.20	0.56
1:B:338:TYR:CD2	1:B:343:VAL:HG12	2.38	0.56
1:B:443:PRO:HA	1:B:446:TRP:CE3	2.41	0.56
1:C:375:PRO:HB2	1:C:378:CYS:SG	2.45	0.56
1:A:315:SER:HB2	2:B:555:HOH:O	2.05	0.56
1:B:453:GLN:O	1:B:454:MET:HB2	2.06	0.56
1:C:345:ALA:HB2	1:C:382:ILE:HD13	1.88	0.56
1:A:282:ARG:HH21	1:A:282:ARG:HG2	1.71	0.55
1:A:400:PHE:HA	1:A:403:VAL:CG1	2.36	0.55
1:A:343:VAL:HG22	1:A:383:PHE:HB3	1.89	0.55
1:D:357:SER:HB3	1:D:360:CYS:HB3	1.88	0.55
1:D:393:ALA:O	1:D:396:VAL:HG12	2.07	0.55
1:A:344:TYR:HB2	2:A:466:HOH:O	2.06	0.55
1:C:364:HIS:HB3	1:C:366:PHE:CE2	2.42	0.55
1:D:275:VAL:HG22	1:D:282:ARG:NH1	2.21	0.55
1:B:401:GLU:HB2	2:B:485:HOH:O	2.06	0.54
1:D:343:VAL:HG22	1:D:383:PHE:CB	2.37	0.54
1:D:400:PHE:HA	1:D:403:VAL:HG12	1.89	0.54
1:C:348:LEU:N	1:C:348:LEU:HD12	2.21	0.54
1:D:320:ASN:HD21	1:D:323:ILE:HG13	1.72	0.54
1:D:433:PRO:HB2	2:D:585:HOH:O	2.08	0.54
1:A:343:VAL:HG23	1:A:382:ILE:CG1	2.38	0.54
1:C:396:VAL:HG13	1:C:397:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:VAL:HG13	1:D:397:ASN:OD1	2.08	0.54
1:A:359:ASN:HD21	1:A:384:ASN:N	2.01	0.54
1:A:457:PRO:O	1:A:460:PRO:HD3	2.08	0.54
1:C:386:GLN:HG2	2:C:484:HOH:O	2.07	0.54
1:D:278:GLU:HA	1:D:433:PRO:O	2.08	0.54
1:B:320:ASN:C	1:B:320:ASN:HD22	2.11	0.53
1:A:454:MET:SD	1:C:332:LYS:HE3	2.47	0.53
1:B:332:LYS:NZ	1:C:459:ASN:H	2.07	0.53
1:A:334:VAL:HB	1:A:353:ILE:HD13	1.91	0.53
1:B:456:SER:N	1:B:457:PRO:HD3	2.24	0.53
1:A:270:HIS:HA	1:A:289:ALA:O	2.09	0.53
1:A:320:ASN:ND2	1:A:320:ASN:C	2.61	0.53
1:A:337:TYR:HD2	2:A:466:HOH:O	1.91	0.53
1:A:348:LEU:HD12	1:A:348:LEU:N	2.25	0.52
1:A:384:ASN:HD22	1:A:387:GLU:CB	2.22	0.52
1:C:402:THR:HG23	2:C:524:HOH:O	2.09	0.52
1:B:341:GLY:CA	1:B:385:ASN:HD22	2.22	0.52
1:C:385:ASN:HB2	1:C:446:TRP:CZ3	2.44	0.52
1:B:282:ARG:NH2	1:B:282:ARG:HG2	2.23	0.52
1:A:320:ASN:HD21	1:A:322:THR:HG23	1.73	0.52
1:A:354:PHE:HE2	1:A:424:TYR:HH	1.57	0.52
1:A:460:PRO:HA	2:A:530:HOH:O	2.09	0.52
1:C:400:PHE:HA	1:C:403:VAL:HG12	1.91	0.52
1:D:287:PHE:HD1	1:D:304:ASN:ND2	2.08	0.52
1:B:380:LEU:HD12	1:D:423:GLU:OE2	2.10	0.52
1:A:316:ASN:C	1:A:316:ASN:HD22	2.12	0.52
1:B:445:GLN:O	1:B:449:LYS:HD3	2.10	0.52
1:B:278:GLU:CD	1:B:319:ARG:HH21	2.13	0.51
1:C:422:ALA:O	1:C:423:GLU:HB2	2.10	0.51
1:D:335:HIS:HB3	1:D:346:GLU:HB3	1.92	0.51
1:D:355:VAL:HG22	1:D:414:MET:HB3	1.91	0.51
1:C:334:VAL:HG21	2:C:505:HOH:O	2.10	0.51
1:A:445:GLN:O	1:A:448:ASP:HB3	2.11	0.51
1:B:293:SER:OG	1:B:335:HIS:NE2	2.44	0.51
1:B:400:PHE:HA	1:B:403:VAL:HG12	1.92	0.51
1:D:359:ASN:ND2	1:D:383:PHE:HA	2.26	0.51
1:B:301:ASP:OD2	1:B:303:SER:HB2	2.11	0.51
1:C:454:MET:O	1:C:455:GLY:C	2.49	0.51
1:D:306:LYS:CG	1:D:307:ASN:H	2.22	0.51
1:B:275:VAL:HG22	1:B:282:ARG:NH1	2.26	0.50
1:D:451:LEU:C	1:D:453:GLN:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:LYS:HG2	2:D:563:HOH:O	2.11	0.50
1:C:366:PHE:N	1:C:366:PHE:CD2	2.77	0.50
1:C:443:PRO:HA	1:C:446:TRP:CE3	2.47	0.50
1:D:433:PRO:HG2	2:D:585:HOH:O	2.11	0.50
1:C:456:SER:N	1:C:457:PRO:HD2	2.26	0.49
1:B:275:VAL:HG12	1:B:277:TYR:CE2	2.47	0.49
1:C:269:LYS:O	1:C:271:TRP:N	2.43	0.49
1:D:396:VAL:CG1	1:D:397:ASN:H	2.21	0.49
1:C:456:SER:N	1:C:457:PRO:CD	2.76	0.49
1:A:317:VAL:HG22	2:B:481:HOH:O	2.13	0.49
1:A:400:PHE:CA	1:A:403:VAL:HG12	2.43	0.49
1:B:360:CYS:HA	2:B:582:HOH:O	2.13	0.49
1:B:456:SER:N	1:B:457:PRO:CD	2.75	0.49
1:C:311:LEU:HA	1:C:314:LEU:HD12	1.94	0.49
1:A:428:ASP:HB3	2:A:557:HOH:O	2.12	0.48
1:B:460:PRO:C	1:B:461:ILE:HD12	2.34	0.48
1:C:384:ASN:ND2	1:C:387:GLU:CG	2.63	0.48
1:C:461:ILE:CD1	1:C:461:ILE:N	2.74	0.48
1:D:339:VAL:HG13	1:D:339:VAL:O	2.14	0.48
1:A:343:VAL:HG23	1:A:382:ILE:HG12	1.94	0.48
1:A:461:ILE:HD12	1:A:461:ILE:H	1.79	0.48
1:D:450:VAL:O	1:D:453:GLN:HB3	2.14	0.48
1:A:384:ASN:HD22	1:A:387:GLU:HB2	1.79	0.48
1:C:287:PHE:HD1	1:C:304:ASN:ND2	2.12	0.48
1:D:354:PHE:O	1:D:414:MET:HA	2.13	0.48
1:B:355:VAL:HG22	1:B:414:MET:HB3	1.96	0.47
1:A:316:ASN:HD22	1:A:318:ASN:H	1.60	0.47
1:A:345:ALA:HB2	1:A:382:ILE:HD13	1.95	0.47
1:B:270:HIS:HA	1:B:289:ALA:O	2.14	0.47
1:B:400:PHE:O	1:B:403:VAL:HG12	2.14	0.47
1:C:414:MET:HE1	2:C:505:HOH:O	2.14	0.47
1:C:428:ASP:HB2	2:C:565:HOH:O	2.13	0.47
1:C:428:ASP:O	1:C:431:SER:HB3	2.14	0.47
1:C:460:PRO:HB3	1:D:329:HIS:CE1	2.49	0.47
1:C:320:ASN:HD21	1:C:323:ILE:HG13	1.80	0.47
1:C:409:MET:HE1	2:C:507:HOH:O	2.14	0.47
1:D:293:SER:HB3	2:D:558:HOH:O	2.14	0.47
1:B:276:TYR:CD2	1:B:283:VAL:HB	2.49	0.47
1:D:453:GLN:HG3	1:D:453:GLN:O	2.14	0.47
1:A:332:LYS:HE2	1:B:454:MET:SD	2.54	0.47
1:D:278:GLU:HG3	1:D:283:VAL:CG2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:VAL:HG13	1:B:397:ASN:OD1	2.14	0.47
1:A:358:ARG:NH1	2:A:490:HOH:O	2.47	0.47
1:A:364:HIS:HB3	1:A:366:PHE:CE2	2.50	0.46
1:B:440:LEU:HD22	1:B:440:LEU:N	2.30	0.46
1:B:453:GLN:CG	1:B:454:MET:N	2.78	0.46
1:A:355:VAL:HG22	1:A:414:MET:HB3	1.96	0.46
1:B:278:GLU:O	1:B:279:LEU:HB2	2.16	0.46
1:B:411:THR:HG22	1:B:439:HIS:CD2	2.50	0.46
1:A:441:HIS:HA	1:C:302:PRO:HG3	1.97	0.46
1:B:278:GLU:OE2	1:B:327:ARG:HD2	2.16	0.46
1:C:373:LYS:HE2	2:C:532:HOH:O	2.14	0.46
1:B:348:LEU:HD12	1:B:348:LEU:N	2.31	0.46
1:B:421:GLY:N	1:B:427:GLN:O	2.49	0.46
1:D:443:PRO:HA	1:D:446:TRP:CE3	2.50	0.46
1:C:343:VAL:HG23	1:C:382:ILE:CG1	2.45	0.45
1:D:396:VAL:CG1	1:D:397:ASN:N	2.79	0.45
1:A:282:ARG:HG2	1:A:282:ARG:NH2	2.31	0.45
1:B:451:LEU:C	1:B:453:GLN:H	2.18	0.45
1:C:348:LEU:N	1:C:348:LEU:CD1	2.78	0.45
1:D:320:ASN:ND2	1:D:322:THR:HG23	2.31	0.45
1:A:338:TYR:CD2	1:A:343:VAL:HG12	2.52	0.45
1:B:364:HIS:HB3	1:B:366:PHE:CE2	2.52	0.45
1:B:424:TYR:C	1:B:425:HIS:ND1	2.70	0.45
1:B:425:HIS:HB2	1:B:427:GLN:CG	2.46	0.45
1:D:270:HIS:HA	1:D:289:ALA:O	2.16	0.45
1:D:282:ARG:NH2	1:D:282:ARG:CG	2.78	0.45
1:D:304:ASN:HD22	1:D:304:ASN:HA	1.64	0.45
1:B:455:GLY:O	1:B:456:SER:HB3	2.17	0.45
1:B:460:PRO:O	1:B:461:ILE:O	2.34	0.45
1:C:297:ASP:HB2	1:C:331:GLY:O	2.17	0.45
1:D:334:VAL:HG22	1:D:335:HIS:N	2.31	0.45
1:A:379:SER:HB2	2:A:510:HOH:O	2.17	0.45
1:B:358:ARG:HH11	1:B:358:ARG:HG3	1.79	0.45
1:C:344:TYR:CE1	1:C:381:LYS:HB2	2.52	0.45
1:A:348:LEU:CD1	1:A:348:LEU:N	2.80	0.45
1:A:429:VAL:HG22	1:A:435:TRP:CD2	2.53	0.44
1:A:461:ILE:HD12	1:A:461:ILE:N	2.31	0.44
1:B:459:ASN:O	1:B:461:ILE:N	2.50	0.44
1:D:433:PRO:CB	2:D:585:HOH:O	2.65	0.44
1:C:295:LEU:HB2	1:C:308:ARG:HG2	1.98	0.44
1:D:320:ASN:ND2	1:D:323:ILE:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:HIS:HB3	1:C:346:GLU:HB3	1.98	0.44
1:D:276:TYR:CD2	1:D:283:VAL:HB	2.53	0.44
1:A:363:HIS:HB2	1:A:387:GLU:OE1	2.17	0.44
1:B:306:LYS:CG	1:B:307:ASN:H	2.31	0.44
1:C:320:ASN:C	1:C:320:ASN:ND2	2.69	0.44
1:B:316:ASN:HD21	1:B:318:ASN:HB2	1.83	0.44
1:C:306:LYS:HB3	1:C:306:LYS:HE2	1.89	0.44
1:D:395:SER:O	1:D:396:VAL:C	2.55	0.44
1:D:334:VAL:HB	1:D:353:ILE:CD1	2.46	0.44
1:C:354:PHE:CG	1:C:419:GLY:HA2	2.53	0.43
1:A:281:ASN:HB3	2:A:505:HOH:O	2.17	0.43
1:A:285:GLU:HB3	2:A:595:HOH:O	2.18	0.43
1:B:316:ASN:HB3	1:B:319:ARG:HB2	2.00	0.43
1:D:305:ASN:HD21	1:D:306:LYS:CE	2.31	0.43
1:C:461:ILE:HD12	1:D:329:HIS:CG	2.52	0.43
1:A:305:ASN:OD1	1:A:306:LYS:HD2	2.18	0.43
1:C:302:PRO:CA	2:C:500:HOH:O	2.66	0.43
1:D:348:LEU:HD12	1:D:348:LEU:N	2.33	0.43
1:A:413:ARG:HD3	1:A:429:VAL:HG11	1.99	0.43
1:B:278:GLU:HG3	1:B:283:VAL:CG2	2.45	0.43
1:B:384:ASN:ND2	1:B:387:GLU:H	2.16	0.43
1:C:292:THR:HB	1:C:338:TYR:O	2.19	0.43
1:C:385:ASN:HB2	1:C:446:TRP:HZ3	1.83	0.43
1:D:387:GLU:O	1:D:391:LEU:HD23	2.19	0.43
1:A:275:VAL:HG13	1:A:282:ARG:CZ	2.48	0.43
1:B:420:TRP:CE2	1:B:429:VAL:HB	2.54	0.43
1:B:458:HIS:O	1:B:459:ASN:C	2.56	0.43
1:D:320:ASN:ND2	1:D:323:ILE:HG13	2.34	0.43
1:A:316:ASN:HD21	1:A:318:ASN:HB2	1.84	0.43
1:A:354:PHE:O	1:A:414:MET:HA	2.19	0.43
1:D:402:THR:CG2	2:D:581:HOH:O	2.67	0.43
1:B:366:PHE:N	1:B:366:PHE:CD2	2.84	0.42
1:D:301:ASP:OD2	1:D:303:SER:HB2	2.19	0.42
1:C:327:ARG:HH11	1:C:327:ARG:HG2	1.83	0.42
1:A:338:TYR:HD2	1:A:343:VAL:HG12	1.85	0.42
1:C:354:PHE:O	1:C:414:MET:HA	2.20	0.42
1:A:420:TRP:HD1	1:A:427:GLN:O	2.01	0.42
1:B:453:GLN:HG2	1:B:454:MET:N	2.34	0.42
1:C:313:LEU:HD23	1:C:313:LEU:H	1.83	0.42
1:A:297:ASP:HB2	1:A:331:GLY:O	2.19	0.42
1:C:384:ASN:ND2	1:C:386:GLN:HB3	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:O	1:A:343:VAL:HA	2.20	0.42
1:D:297:ASP:HB2	1:D:331:GLY:O	2.19	0.42
1:D:399:GLY:HA3	2:D:599:HOH:O	2.19	0.42
1:C:334:VAL:HG22	1:C:335:HIS:N	2.35	0.42
1:B:343:VAL:CG2	1:B:382:ILE:HG13	2.50	0.42
1:C:395:SER:C	1:C:397:ASN:N	2.74	0.42
1:D:364:HIS:CD2	2:D:575:HOH:O	2.73	0.42
1:D:385:ASN:HB2	1:D:446:TRP:HZ3	1.84	0.42
1:A:316:ASN:ND2	1:A:316:ASN:C	2.74	0.41
1:B:403:VAL:HG11	1:B:453:GLN:NE2	2.31	0.41
1:A:269:LYS:O	1:A:271:TRP:HD1	2.03	0.41
1:B:358:ARG:NH2	2:B:588:HOH:O	2.52	0.41
1:B:416:PHE:O	1:B:417:VAL:HB	2.20	0.41
1:D:326:THR:CB	2:D:585:HOH:O	2.66	0.41
1:A:400:PHE:CD2	1:A:454:MET:HB3	2.55	0.41
1:B:345:ALA:HB2	1:B:382:ILE:HD13	2.01	0.41
1:D:445:GLN:O	1:D:449:LYS:HD3	2.20	0.41
1:B:328:ARG:NH2	2:B:586:HOH:O	2.54	0.41
1:C:278:GLU:CD	1:C:319:ARG:HH21	2.24	0.41
1:C:415:SER:HA	1:C:435:TRP:HA	2.03	0.41
1:D:384:ASN:ND2	1:D:386:GLN:HB3	2.31	0.41
1:D:402:THR:HG23	2:D:581:HOH:O	2.20	0.41
1:A:354:PHE:HE2	1:A:424:TYR:OH	2.03	0.41
1:B:341:GLY:HA2	1:B:385:ASN:HD22	1.85	0.41
1:D:316:ASN:HB3	1:D:319:ARG:HB2	2.02	0.41
1:B:303:SER:HB3	1:B:305:ASN:OD1	2.21	0.41
1:C:312:GLY:C	2:C:586:HOH:O	2.59	0.41
1:C:381:LYS:NZ	2:C:491:HOH:O	2.53	0.41
1:A:381:LYS:HD2	2:A:535:HOH:O	2.19	0.41
1:C:429:VAL:C	1:C:431:SER:H	2.24	0.41
1:A:358:ARG:HH11	1:A:358:ARG:HG3	1.85	0.41
1:B:460:PRO:O	1:B:461:ILE:C	2.60	0.41
1:C:395:SER:O	1:C:397:ASN:N	2.53	0.41
1:D:406:LEU:O	1:D:409:MET:HB2	2.21	0.41
1:A:359:ASN:ND2	1:A:384:ASN:N	2.63	0.41
1:A:422:ALA:O	1:A:423:GLU:HB2	2.21	0.41
1:A:440:LEU:HB3	1:A:443:PRO:HD2	2.02	0.41
1:B:276:TYR:HA	1:B:436:ILE:HG22	2.03	0.41
1:B:354:PHE:O	1:B:414:MET:HA	2.21	0.41
1:A:299:PHE:HB3	1:B:448:ASP:OD2	2.20	0.41
1:C:306:LYS:CG	1:C:307:ASN:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:PHE:HE2	1:C:424:TYR:HH	1.65	0.40
1:D:410:CYS:HB3	1:D:444:LEU:HG	2.02	0.40
1:A:294:VAL:HG22	1:A:336:LEU:HB2	2.03	0.40
1:B:359:ASN:ND2	1:B:383:PHE:HA	2.36	0.40
1:B:411:THR:HA	1:B:438:ILE:O	2.21	0.40
1:B:456:SER:O	1:B:458:HIS:N	2.54	0.40
1:C:275:VAL:HG22	1:C:282:ARG:HH11	1.86	0.40
1:A:406:LEU:O	1:A:409:MET:HB2	2.21	0.40
1:C:343:VAL:CG2	1:C:382:ILE:HG13	2.49	0.40
1:A:304:ASN:HA	1:A:304:ASN:HD22	1.62	0.40
1:B:285:GLU:HB3	2:B:585:HOH:O	2.20	0.40
1:B:304:ASN:HA	1:B:304:ASN:HD22	1.69	0.40
1:B:461:ILE:CD1	1:B:461:ILE:N	2.73	0.40
1:C:329:HIS:HA	2:C:613:HOH:O	2.20	0.40
1:C:302:PRO:HA	2:C:500:HOH:O	2.21	0.40
1:C:294:VAL:CG2	1:C:336:LEU:HB2	2.52	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	196/218 (90%)	176 (90%)	19 (10%)	1 (0%)	29	48
1	B	195/218 (89%)	174 (89%)	13 (7%)	8 (4%)	3	3
1	C	195/218 (89%)	177 (91%)	13 (7%)	5 (3%)	5	8
1	D	182/218 (84%)	169 (93%)	12 (7%)	1 (0%)	29	48
All	All	768/872 (88%)	696 (91%)	57 (7%)	15 (2%)	7	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	VAL
1	B	456	SER
1	B	461	ILE
1	D	396	VAL
1	B	460	PRO
1	C	455	GLY
1	A	269	LYS
1	B	270	HIS
1	C	270	HIS
1	C	460	PRO
1	B	397	ASN
1	B	454	MET
1	C	459	ASN
1	B	457	PRO
1	C	457	PRO

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	178/194 (92%)	164 (92%)	14 (8%)	12	24
1	B	177/194 (91%)	165 (93%)	12 (7%)	16	30
1	C	177/194 (91%)	163 (92%)	14 (8%)	12	24
1	D	165/194 (85%)	152 (92%)	13 (8%)	12	24
All	All	697/776 (90%)	644 (92%)	53 (8%)	13	25

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	306	LYS
1	A	313	LEU
1	A	316	ASN
1	A	320	ASN
1	A	322	THR
1	A	325	ASN

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Mol	Chain	Res	Type
1	A	353	ILE
1	A	391	LEU
1	A	404	TYR
1	A	430	THR
1	A	453	GLN
1	A	454	MET
1	A	461	ILE
1	B	293	SER
1	B	304	ASN
1	B	306	LYS
1	B	311	LEU
1	B	313	LEU
1	B	316	ASN
1	B	320	ASN
1	B	322	THR
1	B	343	VAL
1	B	391	LEU
1	B	428	ASP
1	B	461	ILE
1	C	270	HIS
1	C	304	ASN
1	C	306	LYS
1	C	311	LEU
1	C	313	LEU
1	C	316	ASN
1	C	320	ASN
1	C	322	THR
1	C	353	ILE
1	C	385	ASN
1	C	391	LEU
1	C	420	TRP
1	C	460	PRO
1	C	461	ILE
1	D	293	SER
1	D	304	ASN
1	D	306	LYS
1	D	311	LEU
1	D	313	LEU
1	D	316	ASN
1	D	320	ASN
1	D	322	THR
1	D	353	ILE

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Mol	Chain	Res	Type
1	D	384	ASN
1	D	404	TYR
1	D	428	ASP
1	D	440	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	316	ASN
1	A	318	ASN
1	A	320	ASN
1	A	325	ASN
1	A	359	ASN
1	A	361	ASN
1	A	384	ASN
1	A	386	GLN
1	A	390	GLN
1	A	394	GLN
1	A	397	ASN
1	A	458	HIS
1	A	459	ASN
1	B	281	ASN
1	B	304	ASN
1	B	316	ASN
1	B	320	ASN
1	B	325	ASN
1	B	359	ASN
1	B	361	ASN
1	B	363	HIS
1	B	384	ASN
1	B	385	ASN
1	B	394	GLN
1	B	398	HIS
1	B	453	GLN
1	C	304	ASN
1	C	307	ASN
1	C	316	ASN
1	C	318	ASN
1	C	320	ASN
1	C	359	ASN
1	C	361	ASN

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Mol	Chain	Res	Type
1	C	384	ASN
1	C	397	ASN
1	D	304	ASN
1	D	316	ASN
1	D	320	ASN
1	D	325	ASN
1	D	359	ASN
1	D	361	ASN
1	D	384	ASN
1	D	427	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 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.