Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 02:06 AM EDT

PDB ID	:	2YPF
Title	:	Structure of the AvrBs3-DNA complex provides new insights into the initial thymine-recognition mechanism
Authors	:	Stella, S.; Molina, R.; Yefimenko, I.; Prieto, J.; Silva, G.H.; Bertonati, C.; Juillerat, A.; Duchateau, P.; Montoya, G.
Deposited on	:	2012-10-30
Resolution	:	2.55 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:

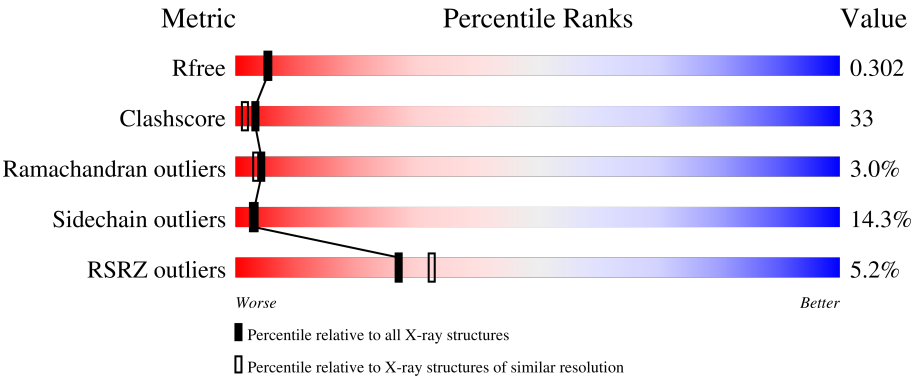
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	758	5%, 41%, 41%, 6% • 11%
2	B	22	5%, 59%, 36%, 5%
3	C	21	5%, 43%, 57%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5822 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 AVRBS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	0	0
			4772	2988	871	897	16			

- Molecule 2 is a DNA chain called 5'-D(*TP*TP*TP*AP*TP*AP*TP*AP*AP*AP*CP*CP *TP*AP *AP*CP*CP*CP*TP*CP*TP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	22	Total	C	N	O	P	0	0	0
			439	214	74	130	21			

- Molecule 3 is a DNA chain called 5'-D(*TP*AP*GP*AP*GP*GP*GP*TP*TP*AP*GP*G P*TP*TP *TP*AP*TP*AP*TP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	P	0	0	0
			436	210	81	125	20			

- Molecule 4 is water.

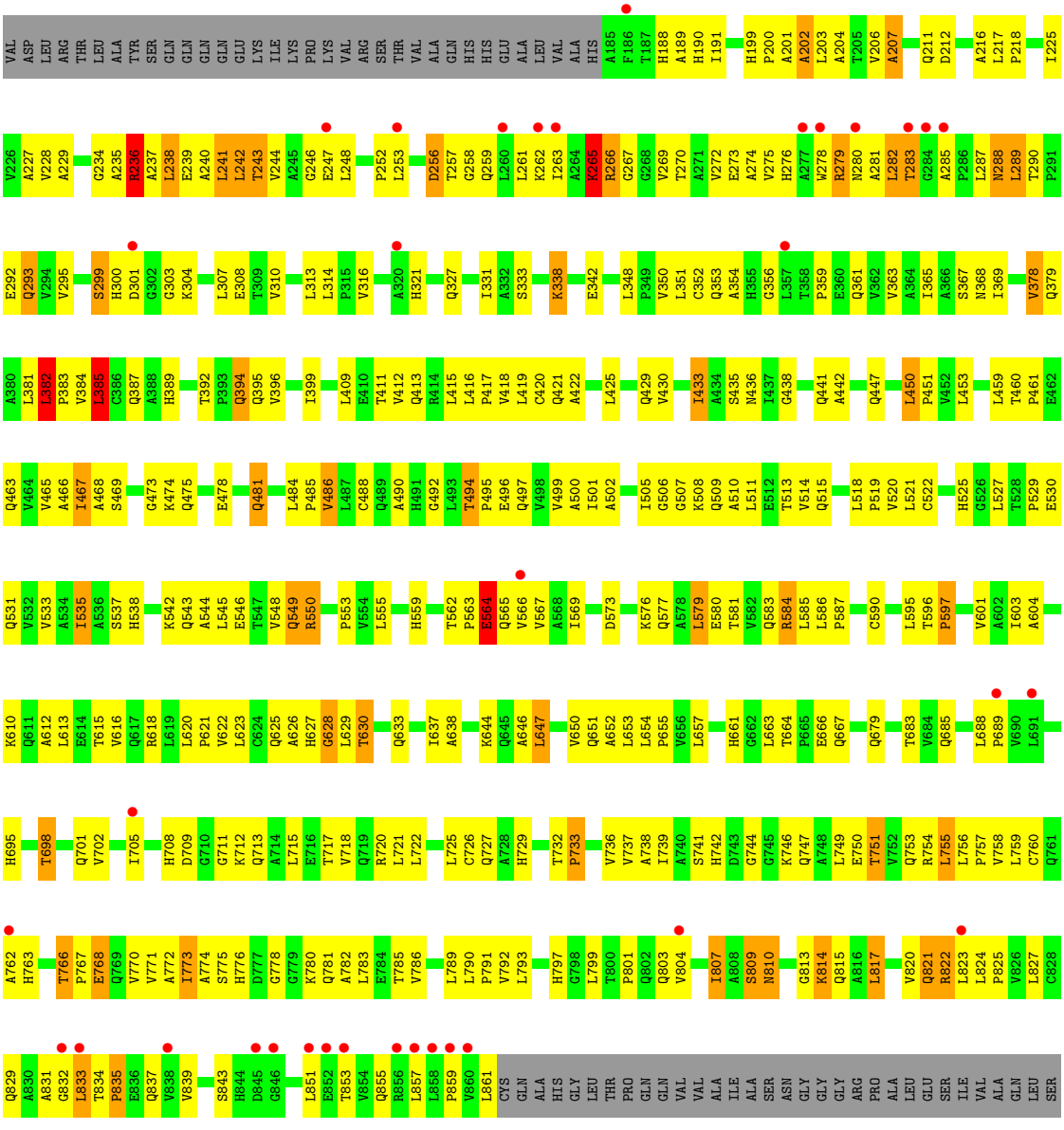
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	17	Total	O	0	0
			17	17		
4	C	19	Total	O	0	0
			19	19		

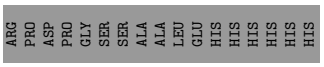
3 Residue-property plots (i)

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: AVRBS3

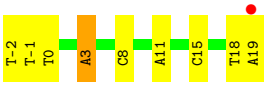
Chain A:





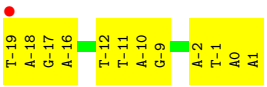
• Molecule 2: 5'-D(*TP*TP*TP*AP*TP*AP*TP*AP*AP*AP*CP*CP*TP*AP *AP*CP*CP*CP*TP*CP*TP*AP)-3'

Chain B:



• Molecule 3: 5'-D(*TP*AP*GP*AP*GP*GP*GP*TP*TP*AP*GP*GP*TP*TP *TP*AP*TP*AP*TP*AP*AP)-3'

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.11Å 100.25Å 61.37Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	32.29 – 2.55 32.29 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.3 (32.29-2.55) 93.3 (32.29-2.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.236 , 0.290 0.246 , 0.302	Depositor DCC
R_{free} test set	1373 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	67.8	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 74.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5822	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.46% 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	0.62	0/4831	0.91	13/6609 (0.2%)
2	B	0.80	1/490 (0.2%)	1.11	1/752 (0.1%)
3	C	0.52	0/490	0.94	0/757
All	All	0.63	1/5811 (0.0%)	0.93	14/8118 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	DA	O3'-P	-7.05	1.52	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	314	LEU	CA-CB-CG	7.26	132.01	115.30
1	A	200	PRO	N-CA-CB	6.35	110.92	103.30
1	A	218	PRO	N-CA-CB	6.16	110.69	103.30
1	A	647	LEU	CB-CG-CD1	-5.97	100.86	111.00
1	A	579	LEU	CB-CG-CD2	-5.58	101.52	111.00
2	B	8	DC	O5'-P-OP2	5.45	117.24	110.70
1	A	419	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	385	LEU	CA-CB-CG	5.28	127.43	115.30
1	A	338	LYS	CD-CE-NZ	-5.26	99.60	111.70
1	A	755	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	628	GLY	N-CA-C	5.23	126.17	113.10
1	A	382	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	861	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	709	ASP	CB-CG-OD1	5.04	122.84	118.30

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	4772	0	4877	347	0
2	B	439	0	252	10	0
3	C	436	0	241	12	0
4	A	139	0	0	35	0
4	B	17	0	0	0	0
4	C	19	0	0	4	0
All	All	5822	0	5370	361	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 33.

All (361) 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:266:ARG:NH1	1:A:267:GLY:H	1.41	1.17
1:A:278:TRP:HB3	1:A:282:LEU:HD21	1.19	1.17
1:A:244:VAL:HB	4:A:2028:HOH:O	1.41	1.17
1:A:604:ALA:HB2	4:A:2104:HOH:O	1.42	1.15
1:A:289:LEU:HB3	1:A:293:GLN:NE2	1.63	1.13
1:A:814:LYS:H	1:A:814:LYS:HD3	1.08	1.10
1:A:289:LEU:HB3	1:A:293:GLN:HE21	1.01	1.10
1:A:266:ARG:HH11	1:A:267:GLY:N	1.48	1.09
1:A:613:LEU:O	1:A:616:VAL:HG12	1.54	1.07
1:A:238:LEU:HD22	1:A:269:VAL:HG22	1.31	1.06
1:A:266:ARG:HD2	2:B:0:DT:H73	1.34	1.05
1:A:531:GLN:O	1:A:535:ILE:HG13	1.57	1.05
1:A:520:VAL:HG23	4:A:2087:HOH:O	1.58	1.03
1:A:814:LYS:HD3	1:A:814:LYS:N	1.76	1.00
1:A:278:TRP:HB3	1:A:282:LEU:CD2	1.92	0.97
1:A:229:ALA:HB3	4:A:2024:HOH:O	1.63	0.96
1:A:497:GLN:O	1:A:501:ILE:HG13	1.65	0.96
1:A:460:THR:CG2	1:A:461:PRO:HD2	1.97	0.95
1:A:488:CYS:O	1:A:492:GLY:HA2	1.67	0.94
3:C:-2:DA:H4'	4:C:2001:HOH:O	1.67	0.94
1:A:266:ARG:HD2	2:B:0:DT:C7	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:THR:HG23	1:A:461:PRO:HD2	1.49	0.93
1:A:295:VAL:O	1:A:299:SER:OG	1.85	0.93
1:A:502:ALA:HB2	1:A:511:LEU:HD11	1.51	0.92
1:A:814:LYS:H	1:A:814:LYS:CD	1.82	0.92
1:A:834:THR:H	1:A:837:GLN:NE2	1.69	0.89
1:A:467:ILE:HD12	1:A:502:ALA:HB1	1.54	0.88
1:A:737:VAL:HG13	1:A:738:ALA:N	1.88	0.88
1:A:825:PRO:O	1:A:829:GLN:HB2	1.73	0.87
1:A:266:ARG:HH11	1:A:267:GLY:H	0.89	0.87
1:A:776:HIS:CD2	1:A:810:ASN:H	1.94	0.86
1:A:238:LEU:HD22	1:A:269:VAL:CG2	2.05	0.85
1:A:708:HIS:HE1	4:A:2124:HOH:O	1.59	0.85
1:A:621:PRO:O	1:A:625:GLN:HG2	1.77	0.84
1:A:307:LEU:O	1:A:310:VAL:HG12	1.79	0.83
1:A:773:ILE:HD11	1:A:783:LEU:HD13	1.59	0.83
1:A:238:LEU:CD2	1:A:269:VAL:HG22	2.08	0.82
1:A:565:GLN:O	1:A:569:ILE:HG13	1.80	0.81
1:A:282:LEU:HD12	1:A:283:THR:OG1	1.79	0.81
1:A:815:GLN:NE2	2:B:15:DC:OP1	2.14	0.81
1:A:781:GLN:HB2	1:A:814:LYS:HG3	1.63	0.79
1:A:616:VAL:O	1:A:620:LEU:HB2	1.82	0.79
1:A:717:THR:OG1	1:A:746:LYS:HG3	1.83	0.79
3:C:-19:DT:H2'	3:C:-18:DA:H5'	1.65	0.79
1:A:727:GLN:HG3	4:A:2129:HOH:O	1.81	0.79
1:A:467:ILE:O	1:A:468:ALA:HB3	1.83	0.79
1:A:713:GLN:O	1:A:746:LYS:HB2	1.83	0.78
1:A:535:ILE:HD11	1:A:567:VAL:HG23	1.67	0.77
1:A:737:VAL:CG1	1:A:738:ALA:N	2.46	0.77
1:A:236:ARG:HG3	1:A:237:ALA:HB2	1.64	0.76
2:B:19:DA:N1	3:C:-19:DT:O4	2.18	0.76
1:A:282:LEU:HD12	1:A:283:THR:N	2.02	0.75
1:A:577:GLN:HB3	1:A:610:LYS:HD3	1.69	0.74
1:A:803:GLN:O	1:A:807:ILE:HG23	1.87	0.74
1:A:289:LEU:CB	1:A:293:GLN:HE21	1.92	0.74
1:A:416:LEU:HG	1:A:430:VAL:HG11	1.70	0.74
1:A:505:ILE:HD11	4:A:2053:HOH:O	1.86	0.74
1:A:785:THR:HG22	1:A:817:LEU:HD23	1.70	0.73
1:A:772:ALA:O	1:A:809:SER:OG	2.04	0.73
1:A:803:GLN:O	1:A:807:ILE:CG2	2.35	0.73
1:A:510:ALA:O	1:A:514:VAL:HG23	1.89	0.73
1:A:266:ARG:HB3	1:A:301:ASP:OD1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:HIS:O	1:A:279:ARG:HB2	1.88	0.73
2:B:18:DT:H2"	2:B:19:DA:O4'	1.89	0.72
1:A:278:TRP:CB	1:A:282:LEU:HD21	2.11	0.72
1:A:546:GLU:HA	1:A:549:GLN:HE22	1.54	0.72
1:A:350:VAL:O	1:A:354:ALA:HB3	1.90	0.72
3:C:1:DA:H5"	4:C:2018:HOH:O	1.90	0.72
1:A:474:LYS:O	1:A:478:GLU:HG3	1.90	0.71
1:A:201:ALA:HA	1:A:202:ALA:C	2.11	0.71
1:A:814:LYS:N	1:A:814:LYS:CD	2.44	0.71
1:A:316:VAL:HG22	1:A:316:VAL:O	1.89	0.70
3:C:-9:DG:H5"	4:C:2008:HOH:O	1.92	0.70
1:A:753:GLN:HG3	1:A:754:ARG:H	1.56	0.70
1:A:460:THR:HG22	1:A:461:PRO:CD	2.21	0.70
1:A:756:LEU:HD13	1:A:770:VAL:HG21	1.74	0.70
1:A:278:TRP:O	1:A:282:LEU:HD11	1.92	0.69
1:A:460:THR:CG2	1:A:461:PRO:CD	2.69	0.69
1:A:781:GLN:CB	1:A:814:LYS:HG3	2.23	0.69
1:A:227:ALA:HB3	4:A:2023:HOH:O	1.92	0.69
1:A:241:LEU:C	1:A:241:LEU:HD12	2.13	0.69
1:A:441:GLN:HB3	1:A:474:LYS:HD3	1.74	0.69
1:A:282:LEU:CD1	1:A:283:THR:N	2.56	0.69
1:A:259:GLN:HE21	1:A:295:VAL:HG21	1.57	0.69
1:A:282:LEU:HA	1:A:287:LEU:HB2	1.76	0.67
1:A:308:GLU:HB3	4:A:2045:HOH:O	1.93	0.67
1:A:276:HIS:CD2	4:A:2028:HOH:O	2.47	0.67
1:A:412:VAL:O	1:A:416:LEU:HB2	1.94	0.67
1:A:266:ARG:CD	2:B:0:DT:C7	2.71	0.67
1:A:782:ALA:HB2	1:A:814:LYS:HD2	1.75	0.67
1:A:679:GLN:O	1:A:712:LYS:HB2	1.94	0.67
1:A:766:THR:HB	1:A:768:GLU:HG3	1.76	0.66
1:A:581:THR:O	1:A:585:LEU:HB2	1.95	0.66
1:A:236:ARG:O	1:A:265:LYS:O	2.13	0.66
1:A:473:GLY:N	4:A:2078:HOH:O	2.30	0.65
1:A:623:LEU:HD21	1:A:651:GLN:HB3	1.78	0.65
1:A:753:GLN:HG3	1:A:754:ARG:N	2.11	0.65
1:A:259:GLN:NE2	1:A:295:VAL:HG21	2.12	0.65
1:A:654:LEU:HB3	1:A:655:PRO:HD2	1.77	0.65
1:A:773:ILE:CD1	1:A:783:LEU:HD13	2.26	0.65
1:A:395:GLN:O	1:A:399:ILE:HG13	1.96	0.64
1:A:544:ALA:O	1:A:548:VAL:HG23	1.98	0.64
1:A:252:PRO:HD2	1:A:279:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ARG:HG3	1:A:550:ARG:HH11	1.61	0.64
1:A:564:GLU:CD	1:A:564:GLU:H	2.01	0.64
1:A:465:VAL:CG1	1:A:465:VAL:O	2.45	0.64
1:A:385:LEU:HD11	1:A:413:GLN:HB3	1.80	0.64
1:A:369:ILE:HG21	2:B:3:DA:N7	2.11	0.64
1:A:465:VAL:O	1:A:465:VAL:HG12	1.96	0.64
1:A:809:SER:O	1:A:810:ASN:HB2	1.98	0.64
1:A:518:LEU:HD23	1:A:522:CYS:SG	2.39	0.63
2:B:11:DA:C2	3:C:-10:DA:C2	2.86	0.63
1:A:613:LEU:HD21	4:A:2104:HOH:O	1.98	0.63
3:C:-11:DT:H5"	4:C:2011:HOH:O	1.98	0.63
1:A:279:ARG:O	1:A:282:LEU:O	2.17	0.63
1:A:653:LEU:O	1:A:657:LEU:HD12	1.99	0.63
1:A:433:ILE:HG13	1:A:433:ILE:O	1.98	0.62
1:A:622:VAL:O	1:A:626:ALA:HB3	1.99	0.62
1:A:266:ARG:NH1	1:A:267:GLY:N	2.20	0.61
1:A:460:THR:HG22	1:A:461:PRO:N	2.16	0.61
1:A:514:VAL:O	1:A:518:LEU:HB2	2.00	0.61
1:A:775:SER:O	1:A:776:HIS:ND1	2.34	0.61
1:A:281:ALA:O	1:A:287:LEU:HD22	2.01	0.60
1:A:216:ALA:HA	1:A:217:LEU:CB	2.30	0.60
1:A:300:HIS:NE2	1:A:333:SER:O	2.34	0.60
1:A:389:HIS:CD2	1:A:417:PRO:HD3	2.37	0.60
1:A:257:THR:O	1:A:261:LEU:HD23	2.02	0.60
1:A:654:LEU:HB3	1:A:655:PRO:CD	2.31	0.60
1:A:266:ARG:C	1:A:266:ARG:HD3	2.22	0.59
1:A:304:LYS:HE2	4:A:2044:HOH:O	2.03	0.59
1:A:822:ARG:HH21	1:A:823:LEU:HD11	1.68	0.59
1:A:513:THR:OG1	1:A:542:LYS:HD2	2.02	0.59
1:A:834:THR:HB	1:A:835:PRO:HD2	1.85	0.59
2:B:-2:DT:H1'	2:B:-1:DT:H5'	1.83	0.59
1:A:775:SER:O	1:A:776:HIS:CG	2.55	0.58
1:A:651:GLN:NE2	1:A:652:ALA:HB2	2.18	0.58
1:A:737:VAL:CG1	1:A:738:ALA:H	2.17	0.58
1:A:417:PRO:O	1:A:421:GLN:HG2	2.03	0.58
1:A:274:ALA:O	1:A:278:TRP:HB2	2.04	0.58
1:A:713:GLN:HB3	1:A:746:LYS:HD2	1.84	0.58
1:A:664:THR:O	1:A:667:GLN:HB2	2.03	0.58
1:A:367:SER:O	1:A:368:ASN:CG	2.42	0.57
1:A:381:LEU:O	1:A:385:LEU:HD22	2.04	0.57
1:A:756:LEU:HB3	1:A:757:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLU:HG3	4:A:2095:HOH:O	2.03	0.57
1:A:367:SER:O	1:A:368:ASN:ND2	2.37	0.57
1:A:813:GLY:N	1:A:814:LYS:HD3	2.19	0.57
1:A:661:HIS:CD2	1:A:688:LEU:HD23	2.39	0.57
1:A:316:VAL:O	1:A:316:VAL:CG2	2.54	0.56
3:C:-19:DT:H2'	3:C:-18:DA:C5'	2.34	0.56
1:A:206:VAL:O	1:A:207:ALA:HB3	2.05	0.56
1:A:650:VAL:O	1:A:654:LEU:HB2	2.06	0.56
1:A:657:LEU:HA	1:A:661:HIS:HB2	1.88	0.56
1:A:809:SER:O	1:A:810:ASN:CB	2.54	0.56
2:B:3:DA:C2	3:C:-2:DA:C2	2.93	0.56
1:A:508:LYS:HG2	1:A:509:GLN:HE21	1.70	0.56
1:A:581:THR:HG21	1:A:610:LYS:HD2	1.87	0.56
1:A:236:ARG:HG3	1:A:237:ALA:CB	2.33	0.56
1:A:637:ILE:HG23	1:A:646:ALA:HB1	1.87	0.56
1:A:718:VAL:O	1:A:722:LEU:N	2.38	0.56
1:A:801:PRO:HA	1:A:804:VAL:CG2	2.36	0.56
1:A:543:GLN:O	1:A:576:LYS:HD2	2.06	0.55
1:A:793:LEU:HB3	1:A:799:LEU:HD12	1.89	0.55
1:A:597:PRO:HG2	4:A:2103:HOH:O	2.05	0.55
1:A:751:THR:HG21	1:A:780:LYS:HA	1.87	0.55
1:A:282:LEU:HB2	1:A:287:LEU:O	2.06	0.55
1:A:522:CYS:HA	1:A:527:LEU:O	2.07	0.55
1:A:521:LEU:HD22	1:A:527:LEU:HD11	1.87	0.55
1:A:273:GLU:HG2	4:A:2034:HOH:O	2.07	0.54
1:A:797:HIS:HE1	1:A:825:PRO:HG3	1.73	0.54
1:A:562:THR:OG1	1:A:565:GLN:HG3	2.07	0.54
1:A:188:HIS:O	1:A:190:HIS:N	2.30	0.54
1:A:622:VAL:HG12	1:A:627:HIS:HE1	1.73	0.54
1:A:750:GLU:O	1:A:753:GLN:HG2	2.08	0.54
1:A:797:HIS:HB3	1:A:824:LEU:HD23	1.90	0.53
3:C:-17:DG:H2"	3:C:-16:DA:OP2	2.07	0.53
1:A:501:ILE:HD13	1:A:514:VAL:HG21	1.90	0.53
1:A:531:GLN:O	1:A:535:ILE:CG1	2.44	0.53
1:A:282:LEU:HA	4:A:2039:HOH:O	2.08	0.53
1:A:509:GLN:HB3	1:A:542:LYS:HD3	1.91	0.53
1:A:580:GLU:O	1:A:584:ARG:HG2	2.08	0.53
1:A:586:LEU:N	1:A:587:PRO:HD2	2.24	0.53
1:A:518:LEU:HB3	1:A:519:PRO:HD3	1.91	0.52
1:A:282:LEU:HD12	1:A:282:LEU:C	2.30	0.52
1:A:399:ILE:HD13	1:A:412:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:N	4:A:2009:HOH:O	2.40	0.52
1:A:241:LEU:C	1:A:241:LEU:CD1	2.77	0.52
1:A:579:LEU:O	1:A:580:GLU:C	2.48	0.52
1:A:786:VAL:O	1:A:790:LEU:HB2	2.09	0.52
1:A:565:GLN:O	1:A:569:ILE:CG1	2.56	0.52
1:A:385:LEU:CD1	1:A:413:GLN:HB3	2.40	0.51
1:A:564:GLU:O	1:A:567:VAL:HG12	2.09	0.51
1:A:705:ILE:HD13	1:A:718:VAL:HG21	1.92	0.51
1:A:853:THR:HG22	1:A:853:THR:O	2.10	0.51
1:A:797:HIS:CE1	1:A:825:PRO:HG3	2.46	0.51
1:A:259:GLN:O	1:A:263:ILE:HG13	2.11	0.50
1:A:615:THR:OG1	1:A:644:LYS:HG3	2.11	0.50
1:A:418:VAL:O	1:A:422:ALA:HB3	2.11	0.50
1:A:351:LEU:HD21	1:A:379:GLN:HB2	1.93	0.50
1:A:637:ILE:CG2	1:A:647:LEU:HD23	2.41	0.50
1:A:382:LEU:N	1:A:383:PRO:CD	2.75	0.50
1:A:832:GLY:C	1:A:833:LEU:HG	2.32	0.50
1:A:246:GLY:HA3	4:A:2029:HOH:O	2.11	0.50
1:A:711:GLY:O	1:A:715:LEU:HG	2.10	0.50
1:A:463:GLN:HE21	1:A:499:VAL:HG21	1.77	0.50
1:A:698:THR:HB	1:A:701:GLN:HB2	1.94	0.50
1:A:713:GLN:HB3	1:A:746:LYS:CD	2.41	0.50
1:A:285:ALA:O	1:A:288:ASN:HA	2.11	0.49
1:A:621:PRO:O	1:A:625:GLN:CG	2.56	0.49
1:A:272:VAL:O	1:A:275:VAL:HG12	2.12	0.49
1:A:827:LEU:HB3	1:A:833:LEU:HD12	1.95	0.49
1:A:630:THR:HG23	1:A:633:GLN:HG3	1.94	0.49
1:A:622:VAL:HG12	1:A:627:HIS:CE1	2.48	0.49
1:A:460:THR:HG22	1:A:461:PRO:HD2	1.77	0.49
1:A:521:LEU:HB3	1:A:527:LEU:HD12	1.94	0.49
1:A:438:GLY:O	1:A:441:GLN:N	2.46	0.49
1:A:657:LEU:HD22	1:A:663:LEU:HD11	1.95	0.49
1:A:803:GLN:HB3	1:A:839:VAL:HG21	1.94	0.49
1:A:389:HIS:HD2	1:A:417:PRO:HD3	1.76	0.49
1:A:713:GLN:C	1:A:746:LYS:HB2	2.33	0.49
1:A:384:VAL:HG12	1:A:384:VAL:O	2.13	0.49
1:A:763:HIS:CG	1:A:790:LEU:HD23	2.48	0.49
1:A:739:ILE:HD11	1:A:771:VAL:HG22	1.95	0.48
1:A:537:SER:O	1:A:538:HIS:CG	2.65	0.48
1:A:338:LYS:O	1:A:342:GLU:HG3	2.12	0.48
1:A:361:GLN:O	1:A:365:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:GLY:N	4:A:2126:HOH:O	2.44	0.48
1:A:256:ASP:C	1:A:258:GLY:H	2.16	0.48
1:A:712:LYS:HE2	1:A:713:GLN:NE2	2.27	0.48
1:A:290:THR:OG1	1:A:293:GLN:HG2	2.13	0.48
1:A:416:LEU:HB3	1:A:417:PRO:HD3	1.95	0.48
1:A:657:LEU:HB3	1:A:663:LEU:HD12	1.95	0.48
1:A:720:ARG:HG2	1:A:721:LEU:HD13	1.95	0.48
1:A:581:THR:HA	1:A:584:ARG:HG2	1.96	0.48
1:A:756:LEU:O	1:A:760:CYS:SG	2.65	0.48
1:A:217:LEU:O	4:A:2013:HOH:O	2.20	0.47
1:A:282:LEU:CD1	1:A:283:THR:OG1	2.57	0.47
1:A:803:GLN:O	1:A:807:ILE:HG22	2.14	0.47
1:A:352:CYS:O	1:A:356:GLY:HA2	2.14	0.47
1:A:459:LEU:CD2	1:A:495:PRO:HB3	2.45	0.47
1:A:378:VAL:O	1:A:382:LEU:HB2	2.15	0.47
1:A:555:LEU:O	1:A:559:HIS:HB2	2.14	0.47
1:A:827:LEU:HA	1:A:831:ALA:HB3	1.96	0.47
1:A:834:THR:O	1:A:837:GLN:HG3	2.13	0.47
1:A:241:LEU:HD12	1:A:241:LEU:O	2.14	0.47
1:A:564:GLU:HA	1:A:567:VAL:HG12	1.97	0.47
1:A:236:ARG:HA	1:A:237:ALA:HA	1.71	0.47
1:A:467:ILE:O	1:A:468:ALA:CB	2.51	0.47
1:A:225:ILE:HA	4:A:2018:HOH:O	2.14	0.47
1:A:630:THR:HG22	1:A:633:GLN:OE1	2.15	0.47
1:A:239:GLU:O	1:A:239:GLU:CD	2.54	0.46
1:A:463:GLN:O	1:A:467:ILE:HG22	2.14	0.46
1:A:281:ALA:O	1:A:282:LEU:HB3	2.14	0.46
1:A:248:LEU:HG	4:A:2028:HOH:O	2.15	0.46
1:A:758:VAL:O	1:A:762:ALA:HB3	2.16	0.46
1:A:201:ALA:HA	1:A:202:ALA:O	2.16	0.46
1:A:550:ARG:HG3	1:A:550:ARG:NH1	2.29	0.46
1:A:603:ILE:HG23	1:A:612:ALA:HB1	1.97	0.46
1:A:382:LEU:HD23	1:A:396:VAL:HG11	1.98	0.46
1:A:564:GLU:CG	4:A:2095:HOH:O	2.64	0.46
1:A:789:LEU:O	1:A:793:LEU:HD12	2.16	0.46
1:A:501:ILE:HG21	1:A:514:VAL:HG21	1.98	0.45
1:A:546:GLU:O	1:A:550:ARG:HB2	2.16	0.45
1:A:742:HIS:CD2	1:A:776:HIS:N	2.84	0.45
1:A:411:THR:O	1:A:415:LEU:HB2	2.16	0.45
1:A:281:ALA:C	1:A:287:LEU:HD13	2.37	0.45
1:A:494:THR:HB	1:A:496:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:O	1:A:243:THR:HG22	2.16	0.45
3:C:-12:DT:H2"	3:C:-11:DT:OP2	2.16	0.45
1:A:774:ALA:O	4:A:2131:HOH:O	2.21	0.45
1:A:822:ARG:HH21	1:A:823:LEU:CD1	2.29	0.45
1:A:855:GLN:O	1:A:859:PRO:HD2	2.17	0.45
1:A:303:GLY:O	1:A:304:LYS:C	2.53	0.45
1:A:433:ILE:HD11	1:A:442:ALA:C	2.38	0.45
1:A:733:PRO:HA	1:A:736:VAL:HB	1.99	0.45
1:A:290:THR:H	1:A:293:GLN:HE21	1.65	0.45
1:A:256:ASP:C	1:A:258:GLY:N	2.70	0.44
1:A:450:LEU:HD23	1:A:451:PRO:N	2.32	0.44
1:A:581:THR:CG2	1:A:610:LYS:HD2	2.47	0.44
1:A:717:THR:HG22	1:A:717:THR:O	2.17	0.44
1:A:790:LEU:HD12	1:A:804:VAL:HG21	1.98	0.44
1:A:241:LEU:CD1	1:A:241:LEU:O	2.66	0.44
1:A:603:ILE:CG2	1:A:612:ALA:HB1	2.48	0.44
1:A:782:ALA:CB	1:A:814:LYS:HD2	2.46	0.44
1:A:484:LEU:O	1:A:485:PRO:C	2.56	0.44
1:A:327:GLN:O	1:A:331:ILE:HG13	2.17	0.44
1:A:266:ARG:O	1:A:301:ASP:HA	2.18	0.44
1:A:499:VAL:HG12	1:A:500:ALA:N	2.30	0.44
3:C:-1:DT:H1'	3:C:0:DA:C8	2.53	0.44
1:A:203:LEU:O	1:A:204:ALA:C	2.56	0.44
1:A:307:LEU:O	1:A:308:GLU:C	2.56	0.44
1:A:475:GLN:HB3	1:A:508:LYS:HD3	2.00	0.44
1:A:545:LEU:HA	1:A:545:LEU:HD23	1.76	0.44
1:A:695:HIS:HB3	1:A:722:LEU:HD23	2.00	0.44
1:A:708:HIS:CE1	1:A:741:SER:O	2.71	0.43
1:A:506:GLY:O	1:A:507:GLY:C	2.56	0.43
1:A:597:PRO:O	1:A:601:VAL:HG23	2.19	0.43
1:A:623:LEU:O	1:A:628:GLY:N	2.51	0.43
1:A:321:HIS:HE1	4:A:2047:HOH:O	2.01	0.43
1:A:529:PRO:O	1:A:533:VAL:HG23	2.18	0.43
1:A:778:GLY:O	1:A:814:LYS:HE3	2.18	0.43
1:A:563:PRO:O	1:A:566:VAL:N	2.51	0.43
1:A:262:LYS:O	1:A:265:LYS:HE2	2.19	0.43
1:A:383:PRO:O	1:A:387:GLN:HG2	2.19	0.43
1:A:399:ILE:O	1:A:399:ILE:HG22	2.18	0.43
1:A:453:LEU:HD21	1:A:481:GLN:HB2	2.00	0.43
1:A:637:ILE:HG21	1:A:647:LEU:HD23	2.01	0.43
1:A:236:ARG:HG2	1:A:266:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:LEU:O	1:A:820:VAL:HG12	2.19	0.43
1:A:300:HIS:CD2	4:A:2042:HOH:O	2.72	0.43
1:A:604:ALA:CB	4:A:2104:HOH:O	2.24	0.43
1:A:683:THR:HG22	1:A:715:LEU:CD1	2.49	0.43
1:A:829:GLN:HG3	4:A:2140:HOH:O	2.18	0.43
1:A:237:ALA:N	4:A:2025:HOH:O	2.40	0.43
1:A:460:THR:CG2	1:A:461:PRO:N	2.81	0.43
1:A:637:ILE:HG23	1:A:646:ALA:CB	2.49	0.43
1:A:683:THR:HG22	1:A:683:THR:O	2.18	0.43
1:A:416:LEU:HD23	1:A:420:CYS:SG	2.59	0.42
1:A:821:GLN:O	1:A:821:GLN:HG2	2.19	0.42
1:A:429:GLN:O	1:A:433:ILE:HG22	2.19	0.42
1:A:573:ASP:OD1	4:A:2092:HOH:O	2.22	0.42
1:A:688:LEU:HD12	1:A:702:VAL:HG21	2.01	0.42
1:A:378:VAL:HG12	1:A:409:LEU:HD11	2.02	0.42
1:A:603:ILE:HG23	1:A:638:ALA:HB1	2.02	0.42
1:A:359:PRO:O	1:A:363:VAL:HG23	2.20	0.41
1:A:466:ALA:C	1:A:467:ILE:O	2.55	0.41
1:A:688:LEU:H	1:A:689:PRO:HD2	1.85	0.41
1:A:518:LEU:CD2	1:A:522:CYS:SG	3.08	0.41
1:A:613:LEU:HD11	4:A:2104:HOH:O	2.20	0.41
1:A:688:LEU:N	1:A:689:PRO:HD2	2.35	0.41
1:A:494:THR:HB	1:A:496:GLU:H	1.85	0.41
1:A:535:ILE:HD12	1:A:548:VAL:HG21	2.02	0.41
1:A:747:GLN:HB3	1:A:780:LYS:HD2	2.02	0.41
1:A:501:ILE:HG22	1:A:501:ILE:O	2.21	0.41
1:A:546:GLU:HA	1:A:549:GLN:NE2	2.29	0.41
1:A:637:ILE:HD13	1:A:650:VAL:HG21	2.02	0.41
1:A:241:LEU:C	1:A:243:THR:N	2.74	0.41
1:A:416:LEU:CD2	1:A:420:CYS:SG	3.08	0.41
1:A:211:GLN:CB	4:A:2008:HOH:O	2.67	0.41
1:A:623:LEU:HA	1:A:627:HIS:ND1	2.36	0.41
1:A:801:PRO:HA	1:A:804:VAL:HG22	2.03	0.41
1:A:486:VAL:O	1:A:490:ALA:HB3	2.20	0.41
1:A:757:PRO:O	1:A:758:VAL:C	2.59	0.41
1:A:385:LEU:O	1:A:389:HIS:HB2	2.20	0.41
1:A:543:GLN:HB2	4:A:2094:HOH:O	2.19	0.41
1:A:590:CYS:HA	1:A:595:LEU:O	2.20	0.41
1:A:721:LEU:O	1:A:725:LEU:HB2	2.20	0.41
1:A:827:LEU:O	1:A:831:ALA:HB3	2.21	0.41
1:A:240:ALA:C	4:A:2027:HOH:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLN:CD	1:A:394:GLN:N	2.74	0.41
1:A:436:ASN:HD21	1:A:469:SER:C	2.24	0.41
1:A:416:LEU:HB3	1:A:417:PRO:CD	2.51	0.41
1:A:420:CYS:HA	1:A:425:LEU:O	2.21	0.40
1:A:280:ASN:C	1:A:282:LEU:H	2.25	0.40
1:A:545:LEU:O	1:A:549:GLN:NE2	2.54	0.40
1:A:265:LYS:HZ1	1:A:299:SER:C	2.25	0.40
1:A:683:THR:HG22	1:A:715:LEU:HD13	2.04	0.40
1:A:234:GLY:O	1:A:236:ARG:N	2.54	0.40
1:A:236:ARG:HG2	1:A:266:ARG:NE	2.37	0.40
1:A:447:GLN:O	1:A:447:GLN:HG3	2.22	0.40
1:A:750:GLU:O	1:A:753:GLN:CG	2.69	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	670/758 (88%)	551 (82%)	99 (15%)	20 (3%)	4 3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ALA
1	A	235	ALA
1	A	236	ARG
1	A	288	ASN
1	A	810	ASN
1	A	191	ILE
1	A	207	ALA
1	A	247	GLU
1	A	189	ALA

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Mol	Chain	Res	Type
1	A	242	LEU
1	A	265	LYS
1	A	282	LEU
1	A	199	HIS
1	A	228	VAL
1	A	564	GLU
1	A	791	PRO
1	A	553	PRO
1	A	733	PRO
1	A	767	PRO
1	A	835	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	483/584 (83%)	414 (86%)	69 (14%)	3 3

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ARG
1	A	238	LEU
1	A	241	LEU
1	A	242	LEU
1	A	243	THR
1	A	253	LEU
1	A	256	ASP
1	A	265	LYS
1	A	266	ARG
1	A	270	THR
1	A	279	ARG
1	A	283	THR
1	A	289	LEU
1	A	292	GLU
1	A	293	GLN

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Mol	Chain	Res	Type
1	A	299	SER
1	A	313	LEU
1	A	348	LEU
1	A	353	GLN
1	A	378	VAL
1	A	382	LEU
1	A	385	LEU
1	A	392	THR
1	A	394	GLN
1	A	433	ILE
1	A	435	SER
1	A	450	LEU
1	A	467	ILE
1	A	481	GLN
1	A	486	VAL
1	A	494	THR
1	A	515	GLN
1	A	525	HIS
1	A	530	GLU
1	A	535	ILE
1	A	549	GLN
1	A	550	ARG
1	A	564	GLU
1	A	583	GLN
1	A	584	ARG
1	A	596	THR
1	A	597	PRO
1	A	618	ARG
1	A	629	LEU
1	A	630	THR
1	A	666	GLU
1	A	685	GLN
1	A	698	THR
1	A	726	CYS
1	A	729	HIS
1	A	732	THR
1	A	749	LEU
1	A	751	THR
1	A	755	LEU
1	A	759	LEU
1	A	766	THR
1	A	768	GLU

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Mol	Chain	Res	Type
1	A	773	ILE
1	A	792	VAL
1	A	807	ILE
1	A	809	SER
1	A	814	LYS
1	A	817	LEU
1	A	821	GLN
1	A	822	ARG
1	A	833	LEU
1	A	843	SER
1	A	851	LEU
1	A	857	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	280	ASN
1	A	288	ASN
1	A	293	GLN
1	A	368	ASN
1	A	389	HIS
1	A	447	GLN
1	A	457	HIS
1	A	463	GLN
1	A	491	HIS
1	A	509	GLN
1	A	515	GLN
1	A	549	GLN
1	A	611	GLN
1	A	640	ASN
1	A	645	GLN
1	A	708	HIS
1	A	797	HIS
1	A	837	GLN

5.3.3 RNA

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	195:LEU	C	197:SER	N	9.14
1	A	193:ALA	C	195:LEU	N	4.52

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	675/758 (89%)	0.18	35 (5%)	27	32	34, 71, 112, 164	0
2	B	22/22 (100%)	-0.38	1 (4%)	33	40	32, 41, 70, 147	0
3	C	21/21 (100%)	-0.29	1 (4%)	30	37	34, 55, 99, 196	0
All	All	718/801 (89%)	0.15	37 (5%)	27	32	32, 70, 115, 196	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	857	LEU	6.6
1	A	832	GLY	5.1
1	A	284	GLY	4.9
1	A	838	VAL	4.8
1	A	859	PRO	4.5
1	A	277	ALA	4.3
1	A	762	ALA	4.1
1	A	858	LEU	4.1
3	C	-19	DT	3.8
1	A	260	LEU	3.6
1	A	247	GLU	3.5
1	A	280	ASN	3.5
1	A	846	GLY	3.4
1	A	357	LEU	3.3
1	A	263	ILE	3.1
1	A	278	TRP	3.1
1	A	860	VAL	3.0
2	B	19	DA	2.9
1	A	285	ALA	2.8
1	A	262	LYS	2.8
1	A	689	PRO	2.8
1	A	852	GLU	2.8
1	A	804	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	566	VAL	2.7
1	A	301	ASP	2.5
1	A	823	LEU	2.4
1	A	851	LEU	2.4
1	A	853	THR	2.4
1	A	705	ILE	2.3
1	A	691	LEU	2.2
1	A	856	ARG	2.2
1	A	320	ALA	2.2
1	A	186	PHE	2.2
1	A	283	THR	2.1
1	A	253	LEU	2.1
1	A	845	ASP	2.1
1	A	833	LEU	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.