



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:49 AM UTC

PDB ID : 1XNV / pdb_00001xnv
Title : Acyl-CoA Carboxylase Beta Subunit from *S. coelicolor* (PccB), apo form #1
Authors : Diacovich, L.; Mitchell, D.L.; Pham, H.; Gago, G.; Melgar, M.M.; Khosla, C.; Gramajo, H.; Tsai, S.-C.
Deposited on : 2004-10-05
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

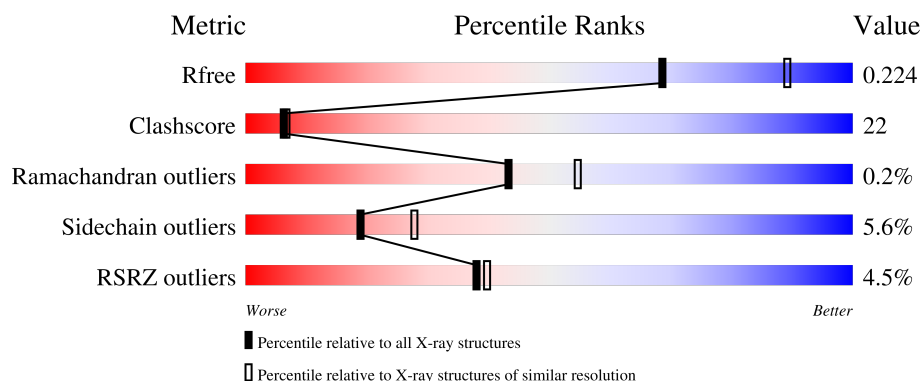
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	530	4% 63% 31% 5%
1	B	530	5% 63% 30% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8611 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 propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	B	521	Total	C	N	O	S	0	0	0
			3952	2480	698	761	13			

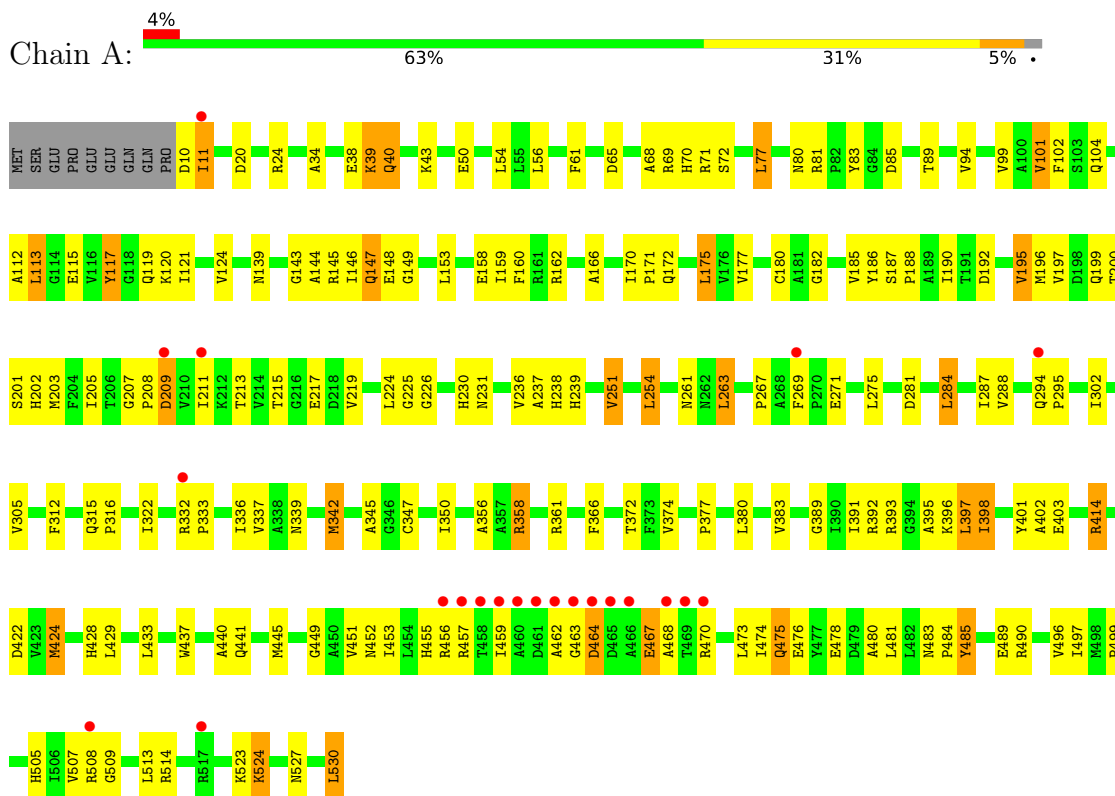
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	352	Total	O	0	0
			352	352		
2	B	354	Total	O	0	0
			354	354		

3 Residue-property plots

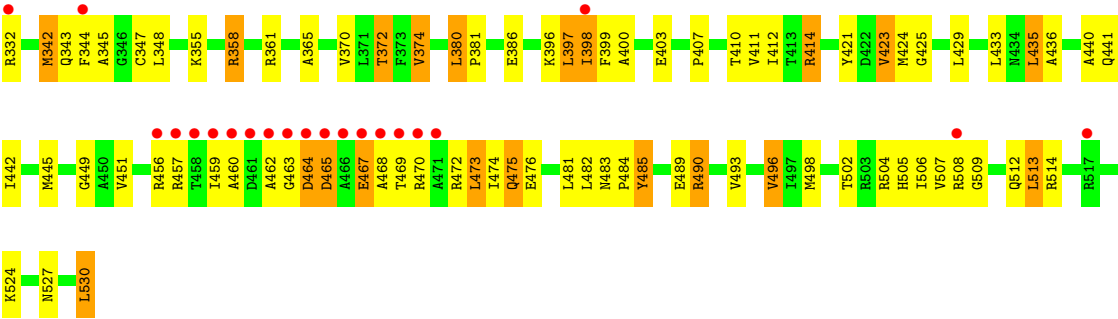
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: propionyl-CoA carboxylase complex B subunit



- Molecule 1: propionyl-CoA carboxylase complex B subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	166.94Å 166.94Å 80.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.25 – 2.30 40.25 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.7 (40.25-2.30) 94.7 (40.25-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	2728 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8611	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.41	0/4033	1.05	21/5478 (0.4%)
1	B	0.41	0/4032	1.07	28/5476 (0.5%)
All	All	0.41	0/8065	1.06	49/10954 (0.4%)

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	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	GLU	N-CA-C	26.78	146.10	112.89
1	B	468	ALA	N-CA-CB	-19.23	80.47	110.28
1	B	467	GLU	N-CA-C	19.14	136.25	111.75
1	A	468	ALA	N-CA-CB	-15.25	86.81	110.30
1	A	467	GLU	CB-CA-C	-10.03	89.04	109.99
1	B	199	GLN	CB-CA-C	-9.82	96.24	111.66
1	A	468	ALA	N-CA-C	-9.67	100.04	112.23
1	A	199	GLN	CB-CA-C	-9.66	96.49	111.66
1	B	464	ASP	CA-C-N	-9.51	108.47	122.07
1	B	464	ASP	C-N-CA	-9.51	108.47	122.07
1	B	414	ARG	N-CA-C	8.76	129.46	110.80
1	A	374	VAL	N-CA-C	8.32	119.82	108.17
1	B	374	VAL	N-CA-C	8.09	119.49	108.17
1	B	464	ASP	N-CA-C	-7.98	98.66	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	TYR	N-CA-C	7.92	120.82	111.71
1	B	467	GLU	O-C-N	-7.80	113.31	122.20
1	B	214	VAL	N-CA-C	7.77	123.31	112.35
1	B	465	ASP	N-CA-CB	-7.64	100.45	111.84
1	B	485	TYR	N-CA-C	7.13	120.09	111.82
1	A	464	ASP	N-CA-C	-6.97	99.57	109.96
1	A	199	GLN	N-CA-C	6.87	120.97	111.90
1	A	463	GLY	N-CA-C	-6.71	104.44	113.24
1	A	414	ARG	N-CA-C	6.65	124.96	110.80
1	B	145	ARG	N-CA-C	-6.58	98.47	108.67
1	A	496	VAL	N-CA-C	-6.16	98.87	107.80
1	A	192	ASP	N-CA-C	6.07	117.97	111.36
1	B	463	GLY	N-CA-C	-6.04	105.33	113.24
1	A	200	THR	N-CA-CB	6.02	123.04	111.07
1	A	94	VAL	N-CA-C	-5.87	99.09	107.77
1	A	524	LYS	N-CA-C	-5.83	105.01	111.36
1	B	213	THR	CB-CA-C	5.73	121.23	110.63
1	B	524	LYS	N-CA-C	-5.67	105.18	111.36
1	A	101	VAL	N-CA-C	5.63	116.47	108.42
1	B	207	GLY	CA-C-N	5.50	124.69	118.97
1	B	207	GLY	C-N-CA	5.50	124.69	118.97
1	B	498	MET	N-CA-C	-5.44	102.93	109.83
1	B	496	VAL	N-CA-C	-5.40	99.96	107.80
1	B	94	VAL	N-CA-C	-5.39	99.79	107.77
1	A	424	MET	N-CA-C	5.34	117.89	109.39
1	B	200	THR	N-CA-CB	5.33	119.50	110.49
1	B	200	THR	N-CA-C	-5.31	99.49	110.80
1	B	465	ASP	N-CA-C	5.28	118.72	111.54
1	A	207	GLY	CA-C-N	5.23	125.28	119.32
1	A	207	GLY	C-N-CA	5.23	125.28	119.32
1	B	414	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	B	469	THR	N-CA-C	-5.09	105.82	111.36
1	A	85	ASP	N-CA-C	5.07	118.58	111.90
1	B	423	VAL	N-CA-C	5.06	115.78	110.62
1	B	192	ASP	N-CA-C	5.05	116.86	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	TYR	Sidechain
1	B	117	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3953	0	3880	182	0
1	B	3952	0	3876	177	0
2	A	352	0	0	66	0
2	B	354	0	0	72	0
All	All	8611	0	7756	347	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 22.

All (347) 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:B:348:LEU:HD11	1:B:424:MET:HE3	1.44	0.99
1:B:295:PRO:HB2	1:B:342:MET:HE3	1.44	0.97
1:A:451:VAL:HG21	1:A:474:ILE:HG12	1.46	0.97
1:B:508:ARG:HD3	1:B:509:GLY:N	1.81	0.95
1:A:508:ARG:HD3	1:A:509:GLY:N	1.88	0.87
1:B:104:GLN:HA	2:B:871:HOH:O	1.75	0.87
1:B:194:THR:HB	2:B:853:HOH:O	1.75	0.87
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.57	0.86
1:A:414:ARG:O	2:A:792:HOH:O	1.92	0.86
1:A:402:ALA:HB1	2:B:882:HOH:O	1.75	0.85
1:A:147:GLN:H	1:A:147:GLN:HE21	1.22	0.85
1:B:145:ARG:O	2:B:719:HOH:O	1.95	0.83
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.61	0.82
1:A:261:ASN:HA	2:A:789:HOH:O	1.79	0.81
1:A:422:ASP:HA	2:A:686:HOH:O	1.81	0.80
1:B:259:PRO:HD3	2:B:777:HOH:O	1.81	0.80
1:A:70:HIS:HD2	1:A:72:SER:H	1.27	0.79
1:A:144:ALA:O	1:A:146:ILE:HD12	1.82	0.79
1:A:483:ASN:HD22	1:A:485:TYR:H	1.30	0.79
1:A:171:PRO:HD3	2:A:789:HOH:O	1.83	0.78
1:A:333:PRO:HG2	2:A:684:HOH:O	1.83	0.78
1:B:345:ALA:O	2:B:814:HOH:O	2.00	0.78
1:A:505:HIS:HA	1:A:508:ARG:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:H	1:A:147:GLN:NE2	1.81	0.76
1:A:437:TRP:HA	2:A:860:HOH:O	1.86	0.75
1:A:71:ARG:HH22	1:A:119:GLN:HE22	1.34	0.75
1:A:451:VAL:HG21	1:A:474:ILE:CG1	2.17	0.74
1:B:197:VAL:HB	2:B:847:HOH:O	1.89	0.73
1:B:485:TYR:O	1:B:489:GLU:HG3	1.88	0.73
1:B:237:ALA:HA	2:B:853:HOH:O	1.88	0.72
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.71	0.72
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.70	0.72
1:B:451:VAL:HG21	1:B:474:ILE:HG12	1.71	0.71
1:B:425:GLY:HA3	2:B:799:HOH:O	1.90	0.71
1:B:85:ASP:HB3	2:B:815:HOH:O	1.90	0.71
1:A:391:ILE:HG23	2:A:704:HOH:O	1.91	0.71
1:B:47:THR:OG1	1:B:50:GLU:HG3	1.90	0.71
1:A:159:ILE:HG12	2:A:770:HOH:O	1.89	0.71
1:A:530:LEU:HG	1:B:396:LYS:HD3	1.73	0.70
1:B:505:HIS:HA	1:B:508:ARG:HD2	1.73	0.70
1:A:361:ARG:HD2	1:A:403:GLU:OE2	1.91	0.70
1:A:202:HIS:HA	2:A:832:HOH:O	1.90	0.70
1:B:445:MET:HE2	1:B:449:GLY:HA3	1.73	0.70
1:A:345:ALA:O	2:A:839:HOH:O	2.08	0.69
1:B:136:VAL:HG23	2:B:820:HOH:O	1.92	0.69
1:A:523:LYS:HD3	2:A:859:HOH:O	1.92	0.69
1:A:524:LYS:HD2	2:B:699:HOH:O	1.92	0.69
2:A:704:HOH:O	1:B:185:VAL:HG23	1.93	0.69
1:B:147:GLN:H	1:B:147:GLN:NE2	1.91	0.68
1:B:483:ASN:HD22	1:B:485:TYR:H	1.41	0.68
1:A:485:TYR:O	1:A:489:GLU:HG3	1.94	0.68
1:B:161:ARG:HG2	2:B:882:HOH:O	1.93	0.67
1:A:459:ILE:HD12	1:A:470:ARG:HD3	1.77	0.67
1:A:505:HIS:O	1:A:508:ARG:NH1	2.25	0.67
1:B:211:ILE:HD11	1:B:219:VAL:HG12	1.76	0.67
1:B:259:PRO:HG2	2:B:873:HOH:O	1.94	0.67
1:B:410:THR:HG22	2:B:848:HOH:O	1.95	0.67
1:B:99:VAL:HG13	2:B:820:HOH:O	1.96	0.66
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.76	0.66
1:B:361:ARG:HD2	1:B:403:GLU:OE2	1.96	0.66
1:A:146:ILE:HD12	1:A:146:ILE:H	1.62	0.65
1:A:499:PRO:HB3	2:A:872:HOH:O	1.95	0.65
1:A:56:LEU:HD12	1:A:61:PHE:HB2	1.79	0.65
1:A:196:MET:HE1	2:A:832:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HB2	2:A:859:HOH:O	1.97	0.64
1:B:436:ALA:HB2	2:B:623:HOH:O	1.98	0.64
1:B:275:LEU:HD23	2:B:760:HOH:O	1.98	0.64
1:B:314:THR:HG23	2:B:669:HOH:O	1.97	0.64
1:B:423:VAL:HG12	1:B:424:MET:HE2	1.78	0.64
1:A:457:ARG:H	1:A:457:ARG:HD2	1.62	0.64
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.62	0.64
1:A:459:ILE:CD1	1:A:470:ARG:HD3	2.29	0.63
1:A:102:PHE:HE2	2:A:749:HOH:O	1.81	0.63
1:A:398:ILE:HD11	1:B:160:PHE:HB3	1.80	0.63
1:B:266:PRO:HB3	2:B:777:HOH:O	1.98	0.63
1:A:315:GLN:N	1:A:316:PRO:HD3	2.13	0.63
1:B:482:LEU:HD13	2:B:860:HOH:O	1.99	0.62
1:B:87:VAL:HB	2:B:871:HOH:O	1.98	0.62
1:A:197:VAL:HB	2:A:729:HOH:O	1.98	0.62
1:A:497:ILE:HG12	2:A:860:HOH:O	2.00	0.62
1:B:70:HIS:HD2	1:B:72:SER:H	1.47	0.62
1:B:200:THR:HA	2:B:684:HOH:O	1.98	0.62
1:B:254:LEU:HD13	2:B:812:HOH:O	2.01	0.61
1:B:508:ARG:HD3	1:B:509:GLY:H	1.64	0.61
1:A:160:PHE:HB3	1:B:398:ILE:HD13	1.82	0.61
1:B:315:GLN:N	1:B:316:PRO:HD3	2.15	0.61
1:A:372:THR:HG21	1:A:401:TYR:OH	2.01	0.61
1:A:480:ALA:C	1:A:481:LEU:HD22	2.25	0.61
1:A:490:ARG:HG3	2:A:647:HOH:O	1.99	0.61
1:B:502:THR:O	1:B:506:ILE:HG12	2.01	0.60
1:B:435:LEU:N	1:B:435:LEU:HD22	2.17	0.60
1:B:71:ARG:HH22	1:B:119:GLN:HE22	1.50	0.60
1:A:147:GLN:HE21	1:A:147:GLN:N	1.98	0.59
1:A:113:LEU:HD22	1:A:117:TYR:CD1	2.36	0.59
1:A:350:ILE:HA	2:A:831:HOH:O	2.00	0.59
1:A:459:ILE:HD12	1:A:470:ARG:HB2	1.84	0.59
2:A:743:HOH:O	1:B:219:VAL:HG21	2.02	0.59
1:A:231:ASN:HD21	1:A:239:HIS:N	2.01	0.59
1:A:345:ALA:C	2:A:839:HOH:O	2.43	0.59
1:B:35:ARG:HG3	2:B:827:HOH:O	2.02	0.59
1:A:295:PRO:HB2	1:A:342:MET:HE3	1.84	0.59
1:B:101:VAL:HB	2:B:789:HOH:O	2.03	0.59
1:B:315:GLN:HB3	2:B:811:HOH:O	2.03	0.58
1:B:175:LEU:HD22	1:B:177:VAL:HG13	1.85	0.58
1:B:414:ARG:O	1:B:441:GLN:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:HIS:ND1	2:B:853:HOH:O	2.33	0.57
1:A:201:SER:HB3	2:A:729:HOH:O	2.04	0.57
1:B:180:CYS:HB3	1:B:203:MET:HG2	1.87	0.57
1:A:77:LEU:HD23	1:A:147:GLN:HG2	1.88	0.56
1:A:395:ALA:O	1:A:398:ILE:HG23	2.06	0.56
1:B:45:LYS:HG2	1:B:200:THR:CG2	2.36	0.56
1:B:121:ILE:O	1:B:124:VAL:HG12	2.04	0.56
1:B:464:ASP:O	1:B:465:ASP:C	2.43	0.56
1:A:34:ALA:O	1:A:38:GLU:HG3	2.05	0.56
2:A:859:HOH:O	1:B:168:GLY:HA3	2.06	0.56
1:A:145:ARG:HD2	1:A:148:GLU:OE2	2.06	0.56
1:A:347:CYS:SG	1:A:377:PRO:HG2	2.46	0.56
1:A:397:LEU:HD21	2:A:776:HOH:O	2.06	0.56
1:A:428:HIS:HD2	2:A:686:HOH:O	1.88	0.56
1:B:365:ALA:HA	2:B:699:HOH:O	2.06	0.56
1:B:147:GLN:HB3	2:B:730:HOH:O	2.06	0.55
1:B:113:LEU:HD22	1:B:117:TYR:CD1	2.40	0.55
1:B:451:VAL:HG21	1:B:474:ILE:CG1	2.37	0.55
1:A:101:VAL:HG13	2:A:856:HOH:O	2.05	0.55
1:B:318:PHE:HB3	2:B:811:HOH:O	2.06	0.55
1:B:69:ARG:HD3	1:B:81:ARG:O	2.07	0.55
1:A:215:THR:HG22	1:A:217:GLU:HG3	1.89	0.55
1:A:219:VAL:HG13	2:A:848:HOH:O	2.07	0.55
1:B:496:VAL:HG21	2:B:786:HOH:O	2.06	0.55
1:A:208:PRO:HG3	2:A:848:HOH:O	2.08	0.54
1:A:392:ARG:HG3	2:A:742:HOH:O	2.07	0.54
1:B:318:PHE:HD2	2:B:811:HOH:O	1.90	0.54
1:A:456:ARG:HD2	1:A:457:ARG:NH1	2.22	0.54
1:B:505:HIS:O	1:B:508:ARG:NH1	2.32	0.54
1:B:145:ARG:HD2	1:B:148:GLU:OE2	2.08	0.54
1:B:472:ARG:O	1:B:476:GLU:HG3	2.08	0.54
1:B:211:ILE:HD11	1:B:219:VAL:CG1	2.37	0.54
1:B:24:ARG:HD3	2:B:737:HOH:O	2.08	0.54
1:B:398:ILE:HG13	1:B:399:PHE:N	2.22	0.54
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.89	0.54
1:B:459:ILE:HD11	1:B:470:ARG:HB2	1.90	0.53
1:A:89:THR:HB	1:A:124:VAL:CG2	2.38	0.53
1:A:398:ILE:HD13	1:A:429:LEU:HD11	1.90	0.53
1:A:437:TRP:HD1	2:A:860:HOH:O	1.90	0.53
1:A:358:ARG:HD3	1:B:527:ASN:HD21	1.72	0.53
1:B:113:LEU:HD22	1:B:117:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:866:HOH:O	1:B:224:LEU:HD12	2.08	0.53
1:B:231:ASN:HD21	1:B:239:HIS:N	2.06	0.53
1:A:414:ARG:O	1:A:441:GLN:N	2.41	0.53
1:A:457:ARG:HD2	1:A:457:ARG:N	2.23	0.53
1:B:159:ILE:HA	2:B:745:HOH:O	2.07	0.53
1:B:332:ARG:HD3	1:B:514:ARG:NH2	2.23	0.53
1:A:153:LEU:HB3	2:B:874:HOH:O	2.07	0.53
1:A:113:LEU:HD22	1:A:117:TYR:CE1	2.44	0.53
2:A:824:HOH:O	1:B:154:GLY:HA3	2.08	0.52
1:B:457:ARG:HB2	2:B:740:HOH:O	2.08	0.52
1:B:230:HIS:HB3	1:B:236:VAL:CG2	2.40	0.52
1:B:398:ILE:HG22	1:B:423:VAL:HG22	1.90	0.52
1:B:483:ASN:HB2	1:B:484:PRO:HD2	1.92	0.52
1:A:332:ARG:HD3	1:A:514:ARG:NH2	2.25	0.52
1:B:200:THR:HG21	2:B:534:HOH:O	2.09	0.52
1:A:70:HIS:CD2	1:A:72:SER:H	2.18	0.52
1:A:254:LEU:HD13	1:A:312:PHE:HE2	1.75	0.52
1:B:355:LYS:HD2	2:B:811:HOH:O	2.08	0.52
1:A:474:ILE:O	1:A:478:GLU:HG2	2.09	0.52
1:A:481:LEU:HD22	1:A:481:LEU:N	2.25	0.52
1:B:238:HIS:HA	1:B:315:GLN:HG2	1.90	0.52
1:A:452:ASN:HD21	1:A:470:ARG:HH11	1.57	0.52
1:A:70:HIS:HE1	1:A:80:ASN:O	1.92	0.51
2:A:857:HOH:O	1:B:224:LEU:HG	2.10	0.51
1:B:319:ALA:HB1	2:B:725:HOH:O	2.09	0.51
1:B:21:LEU:O	1:B:25:ILE:HG22	2.11	0.51
1:A:166:ALA:HB1	2:A:873:HOH:O	2.10	0.51
1:A:508:ARG:HD3	1:A:508:ARG:C	2.35	0.51
1:B:374:VAL:HG22	1:B:424:MET:HB3	1.93	0.51
1:A:10:ASP:OD2	1:A:11:ILE:HG22	2.11	0.51
1:B:122:VAL:HG22	2:B:745:HOH:O	2.10	0.50
1:A:99:VAL:HB	2:A:818:HOH:O	2.11	0.50
1:A:149:GLY:HA3	2:A:768:HOH:O	2.10	0.50
1:A:69:ARG:HD3	1:A:83:TYR:CD2	2.46	0.50
1:A:452:ASN:HD21	1:A:470:ARG:HD2	1.77	0.50
1:B:421:TYR:HD2	2:B:874:HOH:O	1.94	0.50
1:A:497:ILE:CG1	2:A:860:HOH:O	2.56	0.49
1:A:121:ILE:HG22	2:A:770:HOH:O	2.11	0.49
1:A:396:LYS:HD3	1:B:530:LEU:HG	1.94	0.49
1:A:414:ARG:HB2	2:A:775:HOH:O	2.11	0.49
1:A:459:ILE:CD1	1:A:470:ARG:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASP:O	1:A:213:THR:HG23	2.12	0.49
1:A:398:ILE:CD1	1:B:160:PHE:HB3	2.41	0.49
1:A:455:HIS:O	1:A:459:ILE:HG22	2.12	0.49
1:A:505:HIS:HA	1:A:508:ARG:CD	2.41	0.49
1:B:70:HIS:HE1	1:B:80:ASN:O	1.94	0.49
1:B:112:ALA:HA	1:B:143:GLY:O	2.13	0.49
1:B:507:VAL:HG11	2:B:837:HOH:O	2.12	0.49
1:A:196:MET:CE	2:A:832:HOH:O	2.59	0.49
1:A:170:ILE:HG13	2:A:873:HOH:O	2.13	0.49
1:A:337:VAL:O	1:A:372:THR:HA	2.13	0.49
1:B:481:LEU:HB2	2:B:860:HOH:O	2.12	0.49
1:A:284:LEU:O	1:A:287:ILE:HG22	2.12	0.49
1:B:273:ALA:HB3	2:B:837:HOH:O	2.13	0.49
1:A:208:PRO:HA	1:A:211:ILE:HD11	1.93	0.49
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.78	0.48
1:A:195:VAL:HG11	1:A:251:VAL:HG12	1.94	0.48
1:A:230:HIS:HB3	1:A:236:VAL:CG2	2.43	0.48
1:A:505:HIS:O	1:A:508:ARG:HD3	2.14	0.48
1:B:116:VAL:HG12	2:B:815:HOH:O	2.13	0.48
1:B:231:ASN:HD21	1:B:239:HIS:CA	2.26	0.48
1:A:170:ILE:HA	2:A:789:HOH:O	2.13	0.48
1:B:380:LEU:HD23	1:B:381:PRO:HD2	1.95	0.48
1:A:180:CYS:HB3	1:A:203:MET:HG2	1.94	0.48
1:A:302:ILE:O	1:A:305:VAL:HG22	2.14	0.48
1:B:508:ARG:HD3	1:B:508:ARG:C	2.38	0.48
1:B:254:LEU:HB2	2:B:812:HOH:O	2.12	0.48
1:A:231:ASN:HD21	1:A:239:HIS:CA	2.26	0.48
1:B:45:LYS:HG2	1:B:200:THR:HG23	1.96	0.48
1:B:484:PRO:C	2:B:786:HOH:O	2.56	0.48
1:B:158:GLU:O	1:B:162:ARG:HG2	2.14	0.48
1:A:146:ILE:HD12	1:A:146:ILE:N	2.29	0.47
1:A:275:LEU:HD21	1:A:507:VAL:HG11	1.96	0.47
1:A:337:VAL:HG11	2:A:776:HOH:O	2.14	0.47
1:B:201:SER:HB3	2:B:847:HOH:O	2.13	0.47
1:B:230:HIS:HB3	1:B:236:VAL:HG22	1.95	0.47
1:A:527:ASN:HD21	1:B:358:ARG:HD3	1.78	0.47
1:B:411:VAL:C	2:B:848:HOH:O	2.57	0.47
1:A:267:PRO:HG2	2:A:684:HOH:O	2.14	0.47
1:B:74:ASN:HB2	2:B:730:HOH:O	2.15	0.47
1:A:398:ILE:HD12	1:A:398:ILE:O	2.14	0.47
1:B:161:ARG:NH1	2:B:543:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:O	1:A:162:ARG:HG2	2.16	0.46
1:A:524:LYS:HB2	2:B:699:HOH:O	2.14	0.46
1:B:10:ASP:N	2:B:824:HOH:O	2.48	0.46
1:A:68:ALA:O	1:A:69:ARG:HG2	2.15	0.46
1:B:175:LEU:HD23	1:B:195:VAL:HG13	1.98	0.46
1:B:412:ILE:HG21	2:B:867:HOH:O	2.15	0.46
1:A:281:ASP:O	1:A:284:LEU:HB2	2.15	0.46
1:A:424:MET:HE3	2:A:841:HOH:O	2.15	0.46
1:A:451:VAL:CG2	1:A:474:ILE:HG12	2.32	0.46
1:B:493:VAL:HG13	2:B:856:HOH:O	2.15	0.46
1:B:100:ALA:HB1	1:B:124:VAL:CG2	2.45	0.46
1:A:69:ARG:HD2	1:A:81:ARG:O	2.16	0.46
1:A:238:HIS:HA	1:A:315:GLN:HG2	1.97	0.46
1:B:230:HIS:HA	1:B:234:SER:OG	2.16	0.46
1:B:462:ALA:O	1:B:464:ASP:O	2.35	0.45
1:B:440:ALA:O	1:B:483:ASN:HA	2.16	0.45
1:B:101:VAL:HG22	1:B:102:PHE:N	2.31	0.45
1:A:39:LYS:O	1:A:43:LYS:HG3	2.16	0.45
1:B:445:MET:HE2	1:B:449:GLY:CA	2.45	0.45
1:A:177:VAL:HA	2:A:729:HOH:O	2.16	0.45
1:A:295:PRO:HB2	1:A:342:MET:CE	2.46	0.45
1:A:437:TRP:CH2	2:A:872:HOH:O	2.56	0.45
1:A:50:GLU:O	1:A:54:LEU:HD13	2.16	0.45
1:A:236:VAL:HG23	1:A:237:ALA:N	2.31	0.45
1:B:141:SER:O	1:B:179:PRO:HB2	2.17	0.45
1:A:56:LEU:HD22	2:A:818:HOH:O	2.16	0.45
1:A:186:TYR:O	1:A:190:ILE:HG12	2.17	0.45
1:A:225:GLY:N	2:A:843:HOH:O	2.49	0.45
1:A:224:LEU:HD11	1:B:386:GLU:HG3	1.98	0.44
1:A:288:VAL:HG11	2:A:775:HOH:O	2.17	0.44
2:A:857:HOH:O	1:B:204:PHE:HB3	2.16	0.44
1:B:177:VAL:HA	2:B:847:HOH:O	2.17	0.44
1:B:165:HIS:CD2	2:B:882:HOH:O	2.71	0.44
1:B:347:CYS:N	2:B:814:HOH:O	2.50	0.44
1:A:452:ASN:ND2	1:A:470:ARG:HH11	2.15	0.44
1:B:414:ARG:HA	1:B:440:ALA:HA	1.98	0.44
2:A:743:HOH:O	1:B:224:LEU:HA	2.16	0.44
1:A:267:PRO:HD2	2:A:684:HOH:O	2.18	0.44
1:A:445:MET:HE2	1:A:449:GLY:C	2.43	0.44
1:B:275:LEU:HD22	1:B:504:ARG:HA	1.99	0.44
1:B:374:VAL:HG23	2:B:848:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HB3	1:A:188:PRO:CD	2.38	0.43
1:A:339:ASN:ND2	2:A:569:HOH:O	2.35	0.43
1:B:91:TYR:CD1	1:B:91:TYR:C	2.95	0.43
1:A:146:ILE:H	1:A:146:ILE:CD1	2.29	0.43
1:A:172:GLN:HG3	2:A:873:HOH:O	2.18	0.43
1:B:303:GLU:O	1:B:309:ALA:HA	2.18	0.43
1:A:139:ASN:HA	2:A:749:HOH:O	2.18	0.43
1:B:456:ARG:O	1:B:459:ILE:HG22	2.18	0.43
1:A:455:HIS:CG	1:A:473:LEU:HD13	2.53	0.43
1:A:182:GLY:O	1:A:185:VAL:HG22	2.19	0.43
1:A:302:ILE:HD13	1:A:336:ILE:HG21	2.00	0.43
1:B:302:ILE:HG13	2:B:884:HOH:O	2.18	0.43
1:A:68:ALA:C	1:A:69:ARG:HG2	2.44	0.43
1:A:467:GLU:N	1:A:467:GLU:OE2	2.51	0.43
1:B:370:VAL:HG12	1:B:372:THR:HG22	2.01	0.43
1:A:271:GLU:O	1:A:271:GLU:HG3	2.19	0.43
1:B:161:ARG:NE	2:B:572:HOH:O	2.45	0.43
1:A:153:LEU:HD13	2:B:874:HOH:O	2.18	0.43
1:A:345:ALA:HB3	2:A:839:HOH:O	2.18	0.43
1:A:505:HIS:O	1:A:508:ARG:CD	2.67	0.42
1:B:442:ILE:HG12	2:B:867:HOH:O	2.19	0.42
1:B:496:VAL:CG2	2:B:786:HOH:O	2.65	0.42
1:B:29:THR:HG22	2:B:821:HOH:O	2.18	0.42
1:A:104:GLN:HG3	2:A:749:HOH:O	2.19	0.42
1:B:407:PRO:HB3	1:B:513:LEU:HB3	2.02	0.42
1:B:475:GLN:HE21	1:B:475:GLN:HB3	1.67	0.42
1:B:200:THR:HB	2:B:847:HOH:O	2.20	0.42
1:A:115:GLU:CD	1:B:490:ARG:HH22	2.28	0.42
1:B:464:ASP:O	1:B:465:ASP:HB2	2.19	0.42
1:B:505:HIS:O	1:B:508:ARG:CD	2.67	0.42
1:A:112:ALA:HA	1:A:143:GLY:O	2.20	0.42
1:A:470:ARG:O	1:A:474:ILE:HG13	2.20	0.42
1:A:226:GLY:HA2	2:A:832:HOH:O	2.20	0.42
1:A:356:ALA:HB1	2:A:776:HOH:O	2.19	0.42
1:B:40:GLN:OE1	1:B:45:LYS:HE2	2.19	0.42
1:B:485:TYR:HA	2:B:786:HOH:O	2.17	0.42
1:A:269:PHE:HD2	2:A:650:HOH:O	2.03	0.42
1:A:347:CYS:SG	2:A:839:HOH:O	2.59	0.42
1:A:261:ASN:OD1	1:A:263:LEU:HB2	2.20	0.41
1:B:473:LEU:HD12	1:B:473:LEU:HA	1.90	0.41
1:A:89:THR:HB	1:A:124:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLN:O	1:B:344:PHE:C	2.63	0.41
1:B:505:HIS:O	1:B:508:ARG:HD3	2.19	0.41
1:A:226:GLY:C	2:A:832:HOH:O	2.63	0.41
1:B:118:GLY:HA3	1:B:155:ALA:HB1	2.02	0.41
1:B:195:VAL:HG11	1:B:251:VAL:HG12	2.02	0.41
1:B:332:ARG:HH11	1:B:514:ARG:HH21	1.68	0.41
1:A:315:GLN:N	1:A:316:PRO:CD	2.83	0.41
1:A:366:PHE:HE1	2:A:789:HOH:O	2.01	0.41
1:A:452:ASN:ND2	1:A:470:ARG:HD2	2.35	0.41
1:A:453:ILE:HG21	1:B:146:ILE:HD12	2.02	0.41
1:A:475:GLN:HE22	1:A:476:GLU:HG3	1.85	0.41
1:B:345:ALA:C	2:B:814:HOH:O	2.53	0.41
1:B:400:ALA:HB2	2:B:616:HOH:O	2.20	0.41
1:A:440:ALA:O	1:A:483:ASN:HA	2.20	0.41
1:B:231:ASN:HD21	1:B:239:HIS:C	2.27	0.41
1:A:453:ILE:HD12	1:B:146:ILE:CD1	2.50	0.41
1:B:254:LEU:HD13	1:B:312:PHE:HE2	1.86	0.41
1:B:308:ASP:O	1:B:309:ALA:C	2.62	0.41
1:B:136:VAL:HB	2:B:789:HOH:O	2.20	0.41
1:B:490:ARG:HD3	2:B:846:HOH:O	2.20	0.41
1:A:39:LYS:HB3	1:A:39:LYS:NZ	2.36	0.41
1:A:322:ILE:HD13	1:A:356:ALA:HB2	2.02	0.41
1:A:389:GLY:O	1:A:393:ARG:HG3	2.21	0.41
1:A:453:ILE:HD12	1:B:146:ILE:HD11	2.01	0.41
1:A:39:LYS:NZ	1:A:39:LYS:CB	2.84	0.41
1:A:294:GLN:HA	1:A:295:PRO:HD3	1.89	0.41
1:B:147:GLN:H	1:B:147:GLN:HE21	1.64	0.41
1:B:294:GLN:HA	1:B:295:PRO:HD3	1.77	0.41
1:B:512:GLN:HE21	1:B:512:GLN:HB3	1.65	0.40
1:A:20:ASP:O	1:A:24:ARG:HG3	2.22	0.40
1:B:397:LEU:CD1	1:B:424:MET:HE1	2.52	0.40
1:A:383:VAL:HG13	2:A:743:HOH:O	2.21	0.40
1:A:462:ALA:C	1:A:464:ASP:N	2.75	0.40
1:B:209:ASP:OD2	1:B:210:VAL:N	2.55	0.40
1:B:462:ALA:C	1:B:464:ASP:N	2.77	0.40
1:B:208:PRO:O	1:B:211:ILE:HG12	2.21	0.40
1:B:459:ILE:HG23	1:B:460:ALA: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	519/530 (98%)	500 (96%)	18 (4%)	1 (0%)	43	55
1	B	519/530 (98%)	500 (96%)	18 (4%)	1 (0%)	43	55
All	All	1038/1060 (98%)	1000 (96%)	36 (4%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	B	11	ILE

5.3.2 Protein sidechains

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	412/421 (98%)	390 (95%)	22 (5%)	20	30
1	B	412/421 (98%)	388 (94%)	24 (6%)	18	26
All	All	824/842 (98%)	778 (94%)	46 (6%)	19	28

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	40	GLN
1	A	77	LEU
1	A	113	LEU

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Mol	Chain	Res	Type
1	A	147	GLN
1	A	175	LEU
1	A	195	VAL
1	A	205	ILE
1	A	209	ASP
1	A	251	VAL
1	A	254	LEU
1	A	263	LEU
1	A	284	LEU
1	A	342	MET
1	A	358	ARG
1	A	380	LEU
1	A	397	LEU
1	A	398	ILE
1	A	433	LEU
1	A	475	GLN
1	A	513	LEU
1	A	530	LEU
1	B	40	GLN
1	B	77	LEU
1	B	113	LEU
1	B	147	GLN
1	B	161	ARG
1	B	175	LEU
1	B	251	VAL
1	B	263	LEU
1	B	284	LEU
1	B	342	MET
1	B	358	ARG
1	B	372	THR
1	B	380	LEU
1	B	397	LEU
1	B	398	ILE
1	B	429	LEU
1	B	433	LEU
1	B	435	LEU
1	B	467	GLU
1	B	473	LEU
1	B	475	GLN
1	B	490	ARG
1	B	513	LEU
1	B	530	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	40	GLN
1	A	70	HIS
1	A	74	ASN
1	A	119	GLN
1	A	147	GLN
1	A	163	ASN
1	A	199	GLN
1	A	231	ASN
1	A	441	GLN
1	A	448	GLN
1	A	452	ASN
1	A	475	GLN
1	A	483	ASN
1	A	512	GLN
1	A	527	ASN
1	B	30	HIS
1	B	40	GLN
1	B	70	HIS
1	B	74	ASN
1	B	119	GLN
1	B	147	GLN
1	B	163	ASN
1	B	199	GLN
1	B	231	ASN
1	B	299	HIS
1	B	441	GLN
1	B	448	GLN
1	B	475	GLN
1	B	483	ASN
1	B	512	GLN
1	B	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	521/530 (98%)	-0.01	22 (4%) 40 42	21, 32, 59, 113	0
1	B	521/530 (98%)	0.09	25 (4%) 35 37	20, 33, 59, 108	0
All	All	1042/1060 (98%)	0.04	47 (4%) 38 40	20, 32, 59, 113	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	ALA	6.2
1	B	468	ALA	5.5
1	B	465	ASP	5.2
1	A	508	ARG	5.0
1	B	462	ALA	5.0
1	B	508	ARG	5.0
1	B	463	GLY	4.6
1	A	468	ALA	4.6
1	A	462	ALA	4.5
1	A	11	ILE	4.2
1	B	469	THR	3.7
1	A	459	ILE	3.6
1	B	467	GLU	3.6
1	B	458	THR	3.5
1	A	469	THR	3.4
1	A	466	ALA	3.2
1	B	464	ASP	3.1
1	A	211	ILE	3.0
1	A	464	ASP	3.0
1	B	211	ILE	2.9
1	A	463	GLY	2.8
1	B	460	ALA	2.8
1	A	458	THR	2.7
1	A	457	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	460	ALA	2.5
1	B	471	ALA	2.5
1	A	332	ARG	2.5
1	B	459	ILE	2.5
1	B	332	ARG	2.4
1	B	517	ARG	2.4
1	A	269	PHE	2.4
1	B	25	ILE	2.3
1	B	398	ILE	2.3
1	A	470	ARG	2.3
1	B	456	ARG	2.3
1	B	457	ARG	2.2
1	B	470	ARG	2.2
1	A	294	GLN	2.2
1	A	465	ASP	2.2
1	B	461	ASP	2.2
1	B	344	PHE	2.2
1	A	517	ARG	2.1
1	B	11	ILE	2.1
1	A	209	ASP	2.1
1	A	456	ARG	2.0
1	B	269	PHE	2.0
1	A	461	ASP	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 oligosaccharides 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.