Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 06:52 PM EDT

PDB ID	:	1XNV
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 (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:

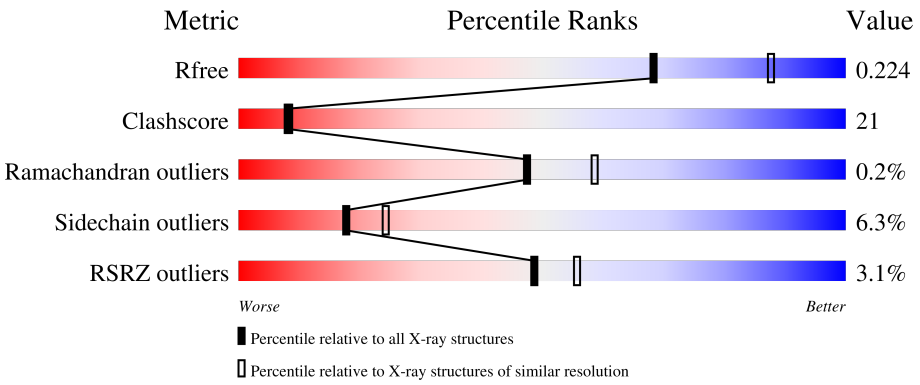
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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% 65% 29% • •
1	B	530	2% 65% 28% • •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	521	3953	2481	698	761	13	0	0	0
1	B	521	3952	2480	698	761	13	0	0	0

- Molecule 2 is water.

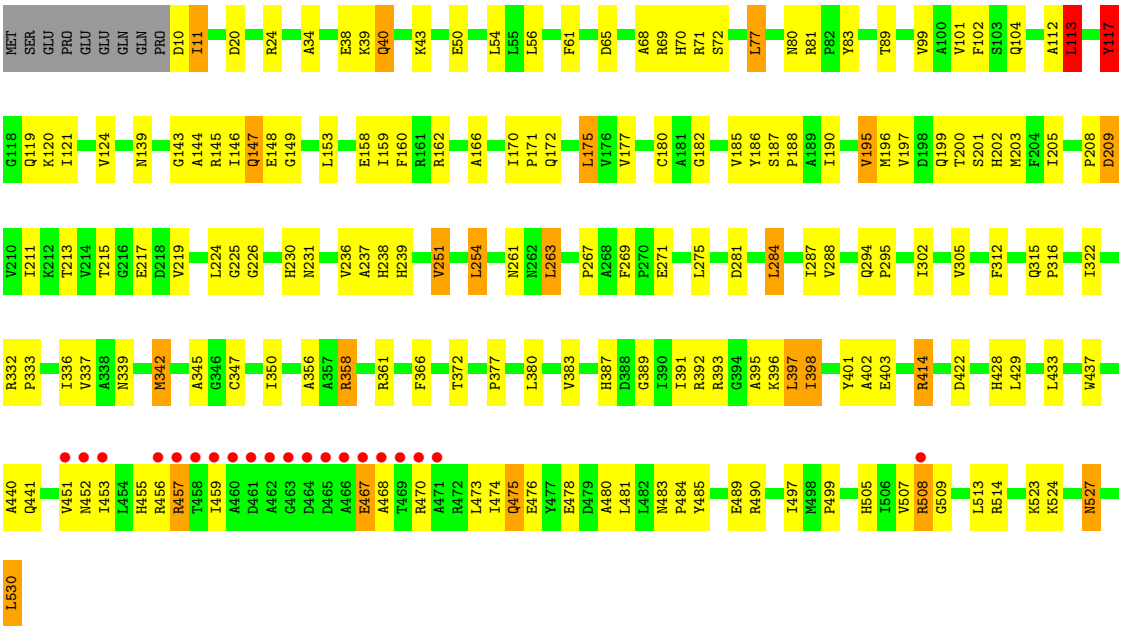
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	352	352	352	0	0
2	B	354	354	354	0	0

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.

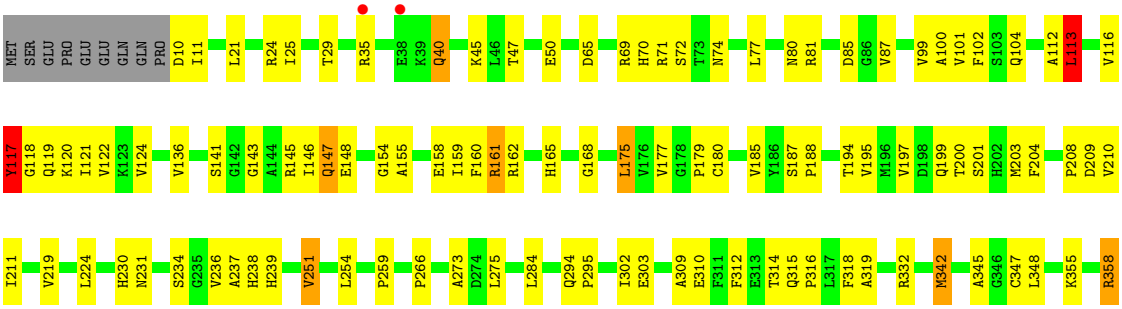
• Molecule 1: propionyl-CoA carboxylase complex B subunit

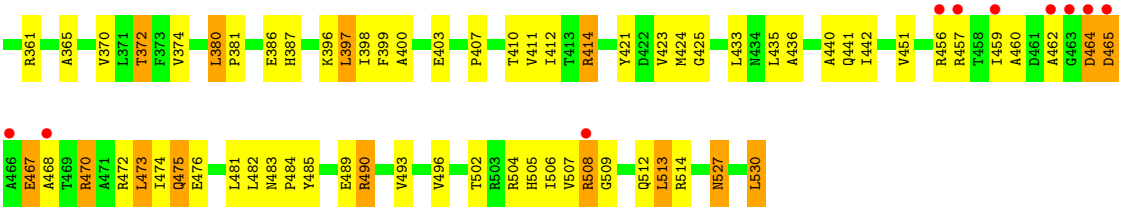
Chain A:



• Molecule 1: propionyl-CoA carboxylase complex B subunit

Chain B:




R361
A365
V370
L371
T372
F373
V374
L380
P381
E386
H387
K396
L397
I398
F399
A400
E403
P407
T410
V411
I412
T413
R414
Y421
D422
V423
M424
G425
L433
N434
L435
A436
A440
Q441
I442
V451
R456
R457
T458
I459
A460
D461
A462
G463
D464
D465
A466
E467
A468
T469
R470
A471
R472
L473
I474
Q475
E476
L481
L482
N483
P484
Y485
E489
R490
V493
V496
T502
R503
R504
H505
I506
V507
R508
G509
Q512
L513
R514
N527
L530

4 Data and refinement statistics (i)

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 70.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.7 (40.25-2.30) 94.8 (70.33-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [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)	0.34 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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	0.34	0/4033	0.72	8/5478 (0.1%)
1	B	0.34	0/4032	0.74	8/5476 (0.1%)
All	All	0.34	0/8065	0.73	16/10954 (0.1%)

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 (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	468	ALA	N-CA-CB	-21.17	80.47	110.10
1	A	468	ALA	N-CA-CB	-16.64	86.81	110.10
1	A	467	GLU	N-CA-C	13.00	146.10	111.00
1	A	467	GLU	CB-CA-C	-10.68	89.04	110.40
1	B	467	GLU	N-CA-C	9.35	136.25	111.00
1	B	199	GLN	CB-CA-C	-7.08	96.24	110.40
1	A	199	GLN	CB-CA-C	-6.95	96.49	110.40
1	B	414	ARG	N-CA-C	6.84	129.46	111.00
1	A	200	THR	N-CA-CB	6.71	123.04	110.30
1	B	467	GLU	O-C-N	-5.87	113.31	122.70
1	A	113	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	465	ASP	N-CA-CB	-5.64	100.45	110.60
1	A	468	ALA	CB-CA-C	5.44	118.27	110.10
1	B	464	ASP	C-N-CA	-5.29	108.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	414	ARG	N-CA-C	5.17	124.96	111.00

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 (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	3953	0	3880	175	0
1	B	3952	0	3876	169	0
2	A	352	0	0	64	0
2	B	354	0	0	71	0
All	All	8611	0	7756	333	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 21.

All (333) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:348:LEU:HD11	1:B:424:MET:HE3	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:B:348:LEU:HD21	1:B:424:MET:HE1	1.80	0.63
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:35:ARG:HG3	2:B:827:HOH:O	2.02	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
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:295:PRO:HB2	1:B:342:MET:HE2	1.86	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:A:480:ALA:C	1:A:481:LEU:HD22	2.25	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: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:A:196:MET:HE1	2:A:832:HOH:O	2.07	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:345:ALA:C	2:A:839:HOH:O	2.43	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:464:ASP:O	1:B:465:ASP:C	2.43	0.54
1:B:505:HIS:O	1:B:508:ARG:NH1	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:PRO:HB2	1:B:342:MET:CE	2.38	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
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:B:374:VAL:HG22	1:B:424:MET:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:348:LEU:HD11	1:B:424:MET:CE	2.39	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
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:B:397:LEU:HD13	1:B:424:MET:HE2	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:508:ARG:HD3	1:A:508:ARG:C	2.35	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: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:A:295:PRO:HB2	1:A:342:MET:CE	2.46	0.45
1:A:177:VAL:HA	2:A:729:HOH:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:B:484:PRO:C	2:B:786:HOH:O	2.56	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: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:411:VAL:C	2:B:848:HOH:O	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:459:ILE:HG23	1:B:460:ALA:N	2.35	0.41
1:B:505:HIS:O	1:B:508:ARG:HD3	2.19	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: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: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: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:A:383:VAL:HG13	2:A:743:HOH:O	2.21	0.40
1:B:209:ASP:OD2	1:B:210:VAL:N	2.55	0.40
1:B:208:PRO:O	1:B:211:ILE:HG12	2.21	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	519/530 (98%)	500 (96%)	18 (4%)	1 (0%)	47	58
1	B	519/530 (98%)	500 (96%)	18 (4%)	1 (0%)	47	58
All	All	1038/1060 (98%)	1000 (96%)	36 (4%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	B	11	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	412/421 (98%)	386 (94%)	26 (6%)	18	24
1	B	412/421 (98%)	386 (94%)	26 (6%)	18	24
All	All	824/842 (98%)	772 (94%)	52 (6%)	18	24

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	77	LEU
1	A	113	LEU
1	A	117	TYR

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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	387	HIS
1	A	397	LEU
1	A	398	ILE
1	A	433	LEU
1	A	457	ARG
1	A	475	GLN
1	A	508	ARG
1	A	513	LEU
1	A	527	ASN
1	A	530	LEU
1	B	40	GLN
1	B	77	LEU
1	B	113	LEU
1	B	117	TYR
1	B	147	GLN
1	B	161	ARG
1	B	175	LEU
1	B	251	VAL
1	B	284	LEU
1	B	310	GLU
1	B	342	MET
1	B	358	ARG
1	B	372	THR
1	B	380	LEU
1	B	387	HIS
1	B	397	LEU
1	B	433	LEU
1	B	467	GLU
1	B	470	ARG
1	B	473	LEU

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Mol	Chain	Res	Type
1	B	475	GLN
1	B	490	ARG
1	B	508	ARG
1	B	513	LEU
1	B	527	ASN
1	B	530	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	387	HIS
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	199	GLN
1	B	231	ASN
1	B	299	HIS
1	B	387	HIS
1	B	448	GLN
1	B	475	GLN
1	B	483	ASN
1	B	512	GLN
1	B	527	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	521/530 (98%)	-0.27	20 (3%)	40	47	21, 32, 59, 113	0
1	B	521/530 (98%)	-0.27	12 (2%)	60	67	20, 33, 59, 108	0
All	All	1042/1060 (98%)	-0.27	32 (3%)	49	56	20, 32, 59, 113	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	ASP	7.7
1	A	462	ALA	6.7
1	A	465	ASP	6.2
1	B	465	ASP	5.6
1	B	464	ASP	5.6
1	B	468	ALA	5.6
1	B	466	ALA	5.0
1	A	468	ALA	4.7
1	A	457	ARG	4.4
1	A	459	ILE	4.3
1	A	466	ALA	4.2
1	A	463	GLY	4.1
1	A	469	THR	4.0
1	B	462	ALA	3.5
1	B	463	GLY	3.4
1	A	460	ALA	3.3
1	B	508	ARG	3.2
1	A	461	ASP	3.0
1	A	508	ARG	2.8
1	A	467	GLU	2.8
1	B	35	ARG	2.8
1	A	458	THR	2.7
1	A	471	ALA	2.6
1	A	470	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	459	ILE	2.5
1	A	453	ILE	2.5
1	A	456	ARG	2.4
1	B	457	ARG	2.3
1	B	456	ARG	2.2
1	B	38	GLU	2.2
1	A	451	VAL	2.1
1	A	452	ASN	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.