



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 09:46 AM UTC

PDB ID : 3PAW / pdb_00003paw
Title : Low resolution X-ray crystal structure of Yeast Rnr1p with dATP bound in the A-site
Authors : Fairman, J.W.; Wijerathna, S.R.; Dealwis, C.G.
Deposited on : 2010-10-19
Resolution : 6.61 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

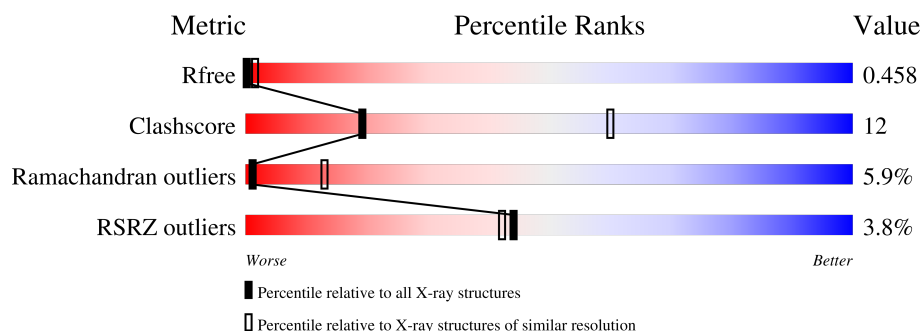
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.61 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	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	888	 3% 67% 16% • 17%
1	B	888	 3% 67% 16% • 17%
1	C	888	 3% 67% 16% • 17%
1	D	888	 3% 69% 14% • 17%

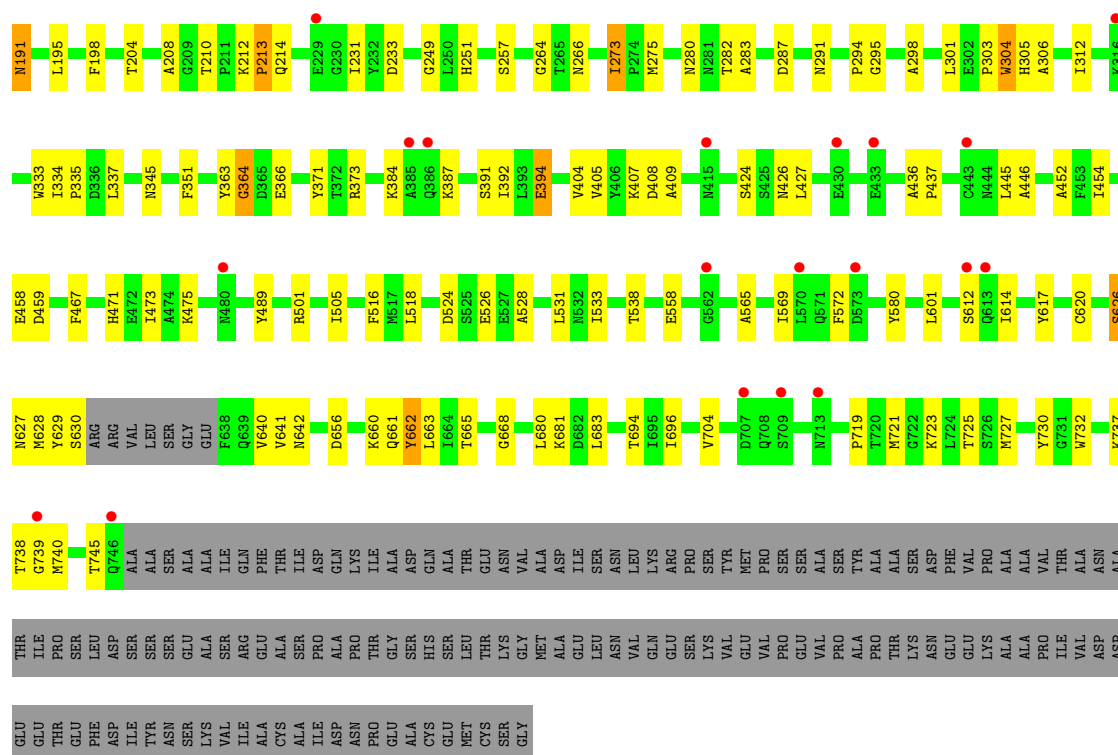
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14596 atoms, of which 0 are hydrogens and 0 are deuteriums.

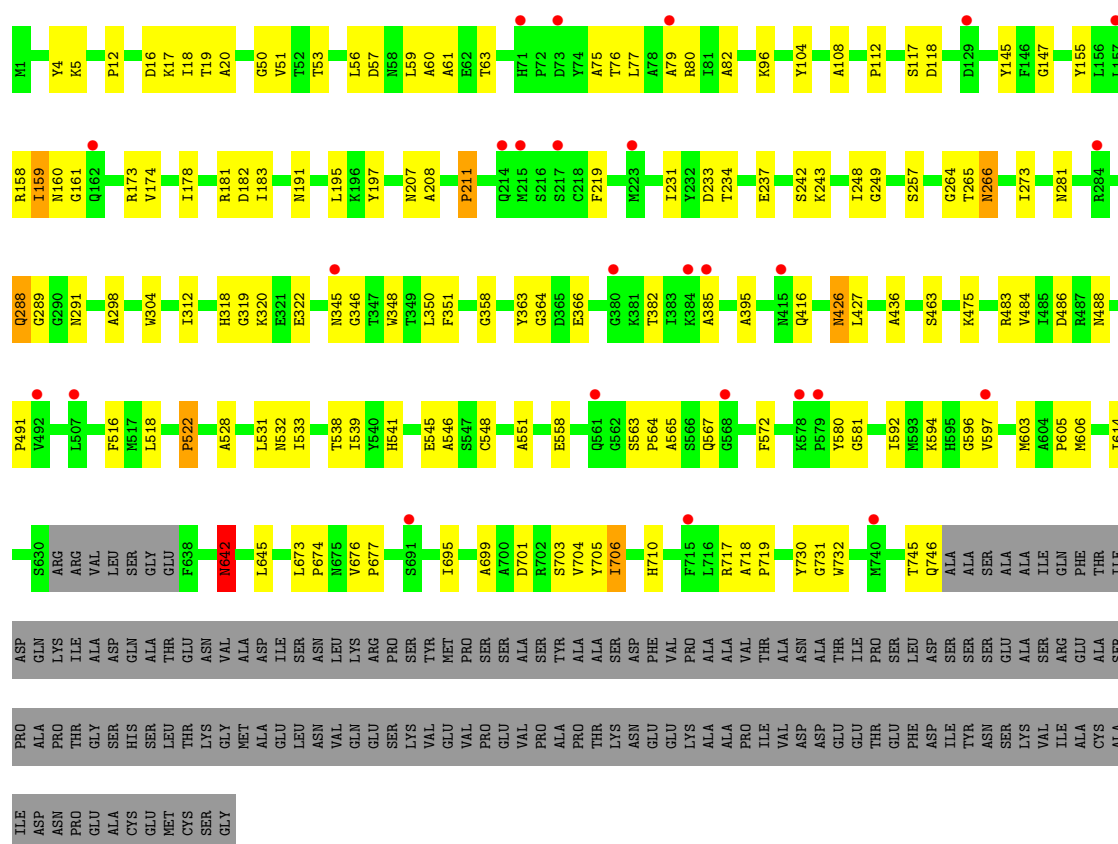
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

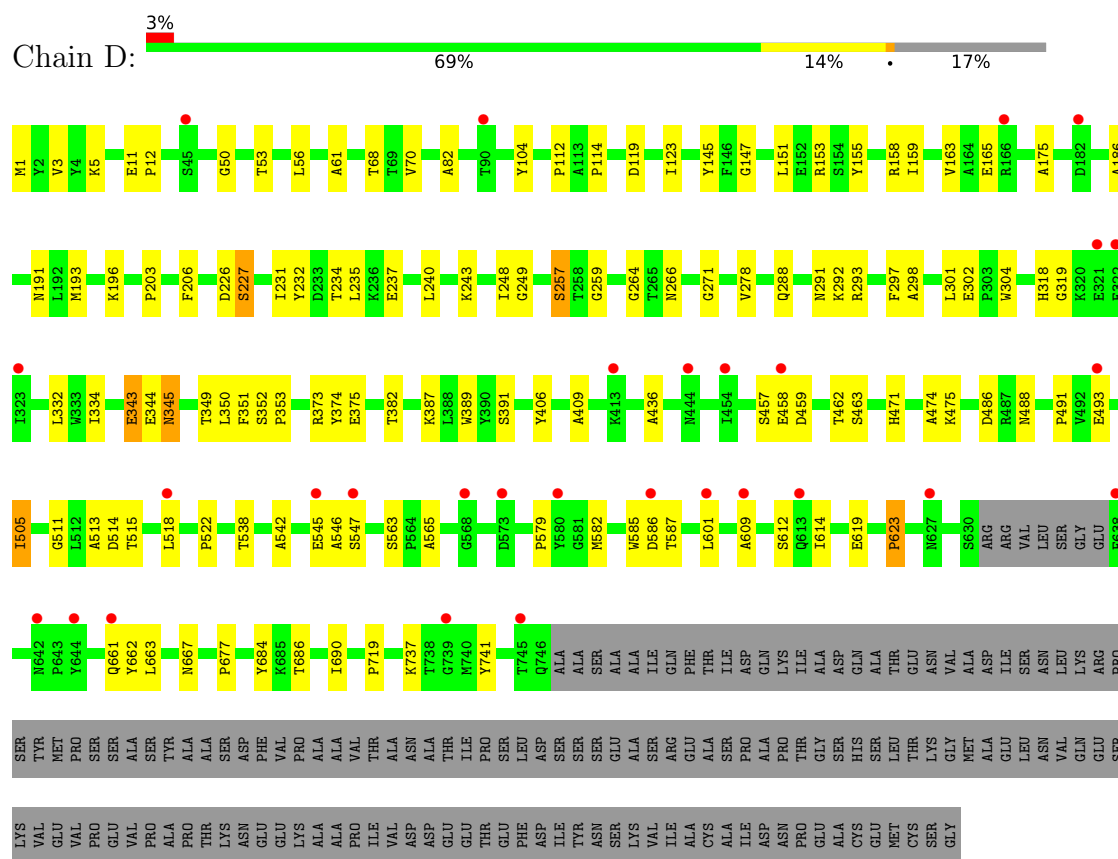
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	739	Total 3649	C 2171	N 739	O 739	0	0	0
1	B	739	Total 3649	C 2171	N 739	O 739	0	0	0
1	C	739	Total 3649	C 2171	N 739	O 739	0	0	0
1	D	739	Total 3649	C 2171	N 739	O 739	0	0	0



• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1



• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	166.51Å 166.51Å 381.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	192.45 – 6.61 190.85 – 6.61	Depositor EDS
% Data completeness (in resolution range)	87.8 (192.45-6.61) 87.7 (190.85-6.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 6.63Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.391 , 0.442 0.392 , 0.458	Depositor DCC
R_{free} test set	469 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	225.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 957.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.437 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14596	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.90	0/3647	1.21	17/5075 (0.3%)
1	B	0.88	0/3647	1.18	16/5075 (0.3%)
1	C	0.91	0/3647	1.20	18/5075 (0.4%)
1	D	0.91	0/3647	1.14	13/5075 (0.3%)
All	All	0.90	0/14588	1.18	64/20300 (0.3%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	642	ASN	CA-C-N	9.29	128.98	118.85
1	B	642	ASN	C-N-CA	9.29	128.98	118.85
1	A	352	SER	CA-C-N	9.05	131.15	119.84
1	A	352	SER	C-N-CA	9.05	131.15	119.84
1	C	695	ILE	N-CA-C	-8.55	104.56	112.43
1	B	39	VAL	N-CA-C	8.00	117.94	111.62
1	A	20	ALA	N-CA-C	-7.35	104.11	113.23
1	D	123	ILE	N-CA-C	-7.13	105.56	111.91
1	A	130	LYS	N-CA-C	-7.07	104.63	113.18
1	B	394	GLU	N-CA-C	-7.01	103.75	112.72
1	B	524	ASP	N-CA-C	6.79	121.22	112.12
1	C	673	LEU	CA-C-N	6.66	126.11	118.85
1	C	673	LEU	C-N-CA	6.66	126.11	118.85
1	A	92	LYS	N-CA-C	6.65	120.26	111.75
1	A	22	ILE	N-CA-C	6.44	116.71	111.62
1	B	291	ASN	N-CA-C	6.34	120.33	112.47
1	C	436	ALA	N-CA-C	6.22	115.47	108.25
1	C	705	TYR	N-CA-C	-5.94	106.06	113.55
1	A	10	LYS	N-CA-C	5.93	117.81	107.49
1	B	334	ILE	N-CA-C	5.92	115.42	108.96
1	C	718	ALA	N-CA-C	5.91	118.03	109.04
1	D	352	SER	CA-C-N	5.91	127.23	119.84
1	D	352	SER	C-N-CA	5.91	127.23	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	612	SER	N-CA-C	5.86	117.67	111.28
1	A	490	TYR	CA-C-N	5.85	125.55	119.05
1	A	490	TYR	C-N-CA	5.85	125.55	119.05
1	D	463	SER	N-CA-C	5.77	117.30	108.42
1	C	358	GLY	N-CA-C	-5.74	107.34	115.43
1	C	385	ALA	N-CA-C	5.73	121.31	113.97
1	B	681	LYS	N-CA-C	-5.72	104.03	111.02
1	C	96	LYS	N-CA-C	-5.57	107.03	113.88
1	A	563	SER	CA-C-N	5.53	126.75	119.84
1	A	563	SER	C-N-CA	5.53	126.75	119.84
1	A	547	SER	N-CA-C	-5.51	106.92	113.97
1	D	436	ALA	CA-C-N	5.50	124.69	118.97
1	D	436	ALA	C-N-CA	5.50	124.69	118.97
1	A	228	ILE	N-CA-C	5.49	116.22	110.62
1	C	642	ASN	CA-C-N	5.47	126.19	120.12
1	C	642	ASN	C-N-CA	5.47	126.19	120.12
1	B	198	PHE	N-CA-C	5.41	116.50	108.60
1	A	359	LEU	N-CA-C	-5.41	106.73	113.38
1	D	505	ILE	N-CA-C	5.41	116.82	108.44
1	A	695	ILE	N-CA-C	-5.33	106.67	112.80
1	C	463	SER	N-CA-C	5.32	117.55	110.53
1	C	118	ASP	N-CA-C	-5.27	106.16	112.59
1	A	524	ASP	N-CA-C	5.25	118.76	107.67
1	B	436	ALA	CA-C-N	5.23	126.38	119.84
1	B	436	ALA	C-N-CA	5.23	126.38	119.84
1	D	302	GLU	CA-C-N	5.21	124.93	119.82
1	D	302	GLU	C-N-CA	5.21	124.93	119.82
1	D	293	ARG	CA-C-N	5.20	125.19	119.89
1	D	293	ARG	C-N-CA	5.20	125.19	119.89
1	C	346	GLY	N-CA-C	5.18	120.28	111.16
1	C	731	GLY	N-CA-C	-5.10	107.34	115.66
1	C	674	PRO	N-CA-C	5.09	120.23	113.40
1	B	662	TYR	N-CA-C	-5.09	106.48	113.30
1	C	158	ARG	N-CA-C	5.08	116.67	108.34
1	D	165	GLU	N-CA-C	5.06	116.88	109.24
1	B	312	ILE	N-CA-C	5.05	118.13	111.17
1	D	387	LYS	N-CA-C	-5.04	106.98	114.64
1	A	118	ASP	N-CA-C	-5.03	107.31	113.50
1	B	384	LYS	N-CA-C	5.03	117.02	110.43
1	C	416	GLN	N-CA-C	5.02	116.48	107.80
1	B	467	PHE	N-CA-C	-5.01	107.33	113.50

There are no chirality outliers.

There are no planarity outliers.

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	3649	0	1652	67	0
1	B	3649	0	1652	68	0
1	C	3649	0	1652	64	0
1	D	3649	0	1652	51	0
All	All	14596	0	6608	249	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 12.

All (249) 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:147:GLY:HA3	1:A:614:ILE:HA	1.42	0.99
1:D:147:GLY:HA2	1:D:614:ILE:HA	1.48	0.95
1:C:603:MET:CB	1:C:706:ILE:HA	1.99	0.92
1:A:147:GLY:CA	1:A:614:ILE:HA	2.02	0.90
1:D:147:GLY:CA	1:D:614:ILE:HA	2.07	0.85
1:D:343:GLU:C	1:D:345:ASN:H	1.84	0.83
1:B:364:GLY:H	1:B:408:ASP:CB	1.94	0.81
1:A:513:ALA:HB2	1:A:623:PRO:HA	1.65	0.78
1:D:515:THR:HA	1:D:518:LEU:CB	2.14	0.77
1:B:660:LYS:C	1:B:662:TYR:H	1.92	0.76
1:C:57:ASP:HA	1:C:60:ALA:HB3	1.69	0.75
1:B:298:ALA:HB3	1:B:427:LEU:HA	1.70	0.74
1:C:147:GLY:CA	1:C:614:ILE:HA	2.18	0.73
1:D:158:ARG:HA	1:D:163:VAL:HA	1.70	0.72
1:D:175:ALA:HB1	1:D:186:ALA:HB1	1.73	0.71
1:C:147:GLY:HA3	1:C:614:ILE:O	1.89	0.71
1:C:147:GLY:HA3	1:C:614:ILE:HA	1.74	0.70
1:C:75:ALA:C	1:C:77:LEU:H	2.00	0.69
1:C:304:TRP:HA	1:C:350:LEU:HA	1.76	0.68
1:D:232:TYR:HA	1:D:235:LEU:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ALA:CB	1:B:427:LEU:HA	2.24	0.67
1:C:242:SER:O	1:C:288:GLN:HA	1.94	0.67
1:B:191:ASN:O	1:B:195:LEU:N	2.28	0.67
1:A:242:SER:O	1:A:288:GLN:HA	1.95	0.66
1:A:27:TYR:C	1:A:29:LEU:H	2.03	0.66
1:C:219:PHE:O	1:C:426:ASN:HA	1.96	0.66
1:B:67:MET:C	1:B:69:THR:H	2.04	0.66
1:D:349:THR:HA	1:D:382:THR:HA	1.77	0.66
1:C:159:ILE:C	1:C:161:GLY:H	2.04	0.65
1:C:563:SER:C	1:C:565:ALA:H	2.04	0.65
1:D:151:LEU:HA	1:D:155:TYR:CB	2.27	0.64
1:D:474:ALA:HB3	1:D:542:ALA:CB	2.27	0.64
1:A:607:PRO:HA	1:A:620:CYS:CB	2.28	0.64
1:A:119:ASP:C	1:A:121:TYR:H	2.07	0.63
1:B:287:ASP:HA	1:B:294:PRO:HA	1.81	0.63
1:C:191:ASN:O	1:C:195:LEU:N	2.26	0.62
1:C:363:TYR:O	1:C:366:GLU:N	2.31	0.62
1:D:1:MET:O	1:D:12:PRO:HA	2.00	0.62
1:B:628:MET:HA	1:B:640:VAL:O	2.00	0.61
1:B:723:LYS:C	1:B:725:THR:H	2.09	0.61
1:D:3:VAL:N	1:D:11:GLU:O	2.34	0.61
1:A:273:ILE:C	1:A:275:MET:H	2.09	0.61
1:B:20:ALA:C	1:B:22:ILE:H	2.08	0.60
1:C:348:TRP:O	1:C:382:THR:HA	2.01	0.60
1:D:304:TRP:O	1:D:350:LEU:HA	2.01	0.60
1:A:2:TYR:HA	1:A:11:GLU:O	2.03	0.59
1:C:16:ASP:O	1:C:20:ALA:HB2	2.02	0.59
1:C:174:VAL:HA	1:C:208:ALA:HB3	1.85	0.59
1:C:248:ILE:O	1:C:298:ALA:N	2.35	0.59
1:C:563:SER:C	1:C:565:ALA:N	2.59	0.59
1:D:474:ALA:HB3	1:D:542:ALA:HB3	1.83	0.59
1:A:217:SER:N	1:A:443:CYS:O	2.35	0.59
1:B:407:LYS:C	1:B:409:ALA:H	2.11	0.58
1:A:198:PHE:CB	1:A:448:VAL:HA	2.32	0.58
1:A:65:ALA:C	1:A:67:MET:H	2.09	0.58
1:B:249:GLY:HA3	1:B:426:ASN:C	2.27	0.58
1:B:627:ASN:N	1:B:668:GLY:HA3	2.18	0.58
1:B:86:LEU:C	1:B:88:LYS:H	2.12	0.58
1:C:484:VAL:O	1:C:488:ASN:CB	2.52	0.57
1:A:280:ASN:HA	1:A:283:ALA:HB3	1.84	0.57
1:C:147:GLY:HA3	1:C:614:ILE:CA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLY:HA3	1:C:614:ILE:C	2.29	0.57
1:D:257:SER:C	1:D:271:GLY:HA2	2.29	0.57
1:B:471:HIS:HA	1:B:538:THR:O	2.04	0.56
1:C:312:ILE:O	1:C:395:ALA:HB1	2.05	0.56
1:C:605:PRO:O	1:C:710:HIS:HA	2.06	0.56
1:D:240:LEU:HA	1:D:243:LYS:CB	2.35	0.56
1:D:104:TYR:O	1:D:112:PRO:HA	2.06	0.56
1:D:343:GLU:C	1:D:345:ASN:N	2.57	0.56
1:A:226:ASP:O	1:A:227:SER:CB	2.55	0.55
1:C:17:LYS:C	1:C:19:THR:H	2.14	0.55
1:A:514:ASP:O	1:A:518:LEU:CB	2.55	0.55
1:D:563:SER:O	1:D:565:ALA:N	2.37	0.54
1:B:725:THR:C	1:B:727:MET:H	2.16	0.54
1:A:375:GLU:C	1:A:377:GLU:H	2.16	0.54
1:C:104:TYR:O	1:C:112:PRO:HA	2.08	0.53
1:A:298:ALA:HA	1:A:329:PHE:O	2.08	0.53
1:B:251:HIS:CB	1:B:424:SER:CB	2.87	0.53
1:C:548:CYS:HA	1:C:597:VAL:HA	1.90	0.53
1:D:612:SER:CB	1:D:619:GLU:HA	2.38	0.53
1:A:147:GLY:HA2	1:A:614:ILE:HA	1.88	0.53
1:C:57:ASP:O	1:C:61:ALA:N	2.36	0.53
1:A:249:GLY:HA2	1:A:298:ALA:O	2.09	0.53
1:B:75:ALA:C	1:B:77:LEU:H	2.15	0.53
1:C:545:GLU:HA	1:C:548:CYS:CB	2.39	0.52
1:A:175:ALA:HB1	1:A:186:ALA:O	2.10	0.52
1:B:20:ALA:C	1:B:22:ILE:N	2.66	0.52
1:D:343:GLU:O	1:D:345:ASN:N	2.42	0.52
1:A:508:GLY:HA3	1:A:605:PRO:HA	1.91	0.52
1:A:523:PHE:H	1:A:683:LEU:HA	1.74	0.52
1:D:514:ASP:O	1:D:518:LEU:N	2.43	0.52
1:D:661:GLN:C	1:D:663:LEU:H	2.18	0.52
1:D:334:ILE:O	1:D:406:TYR:HA	2.10	0.52
1:A:197:TYR:HA	1:A:452:ALA:CB	2.40	0.52
1:B:304:TRP:O	1:B:351:PHE:N	2.42	0.52
1:D:513:ALA:HB2	1:D:623:PRO:HA	1.92	0.52
1:A:224:LYS:O	1:A:225:GLU:CB	2.58	0.51
1:C:572:PHE:N	1:C:704:VAL:O	2.43	0.51
1:B:660:LYS:C	1:B:662:TYR:N	2.62	0.51
1:C:249:GLY:HA2	1:C:298:ALA:O	2.10	0.51
1:B:231:ILE:C	1:B:233:ASP:H	2.17	0.51
1:C:243:LYS:HA	1:C:289:GLY:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:C	1:A:361:ASP:H	2.18	0.51
1:C:61:ALA:HB1	1:C:82:ALA:HB2	1.93	0.51
1:D:226:ASP:O	1:D:227:SER:CB	2.59	0.51
1:A:339:MET:C	1:A:341:ARG:H	2.19	0.51
1:B:721:MET:C	1:B:723:LYS:H	2.18	0.51
1:C:75:ALA:C	1:C:77:LEU:N	2.64	0.50
1:D:234:THR:HA	1:D:237:GLU:CB	2.41	0.50
1:A:196:LYS:O	1:A:449:ALA:HB3	2.12	0.50
1:D:373:ARG:C	1:D:375:GLU:H	2.19	0.50
1:D:147:GLY:HA3	1:D:614:ILE:HA	1.91	0.50
1:B:65:ALA:C	1:B:67:MET:H	2.20	0.50
1:B:363:TYR:O	1:B:366:GLU:N	2.40	0.50
1:B:694:THR:C	1:B:696:ILE:H	2.20	0.49
1:C:298:ALA:HB3	1:C:427:LEU:HA	1.95	0.49
1:A:299:LEU:O	1:A:331:ALA:N	2.41	0.49
1:A:27:TYR:O	1:A:29:LEU:N	2.40	0.49
1:A:60:ALA:C	1:A:62:GLU:N	2.70	0.49
1:A:16:ASP:O	1:A:20:ALA:HB2	2.12	0.49
1:A:60:ALA:C	1:A:62:GLU:H	2.20	0.49
1:A:312:ILE:O	1:A:395:ALA:HB1	2.12	0.49
1:A:538:THR:O	1:A:542:ALA:N	2.46	0.49
1:C:231:ILE:C	1:C:233:ASP:H	2.21	0.49
1:C:531:LEU:C	1:C:533:ILE:H	2.21	0.48
1:B:335:PRO:C	1:B:337:LEU:H	2.20	0.48
1:B:730:TYR:C	1:B:732:TRP:H	2.21	0.48
1:C:117:SER:HA	1:C:211:PRO:HA	1.95	0.48
1:D:474:ALA:HB3	1:D:542:ALA:HB1	1.95	0.48
1:C:77:LEU:HA	1:C:80:ARG:CB	2.44	0.48
1:C:281:ASN:CB	1:D:278:VAL:HA	2.43	0.48
1:D:301:LEU:O	1:D:332:LEU:HA	2.13	0.48
1:D:61:ALA:CB	1:D:82:ALA:HB2	2.42	0.48
1:C:159:ILE:C	1:C:161:GLY:N	2.72	0.48
1:B:392:ILE:C	1:B:394:GLU:H	2.22	0.48
1:B:505:ILE:N	1:B:601:LEU:O	2.41	0.47
1:B:531:LEU:C	1:B:533:ILE:H	2.22	0.47
1:C:173:ARG:O	1:C:208:ALA:O	2.31	0.47
1:A:52:THR:O	1:A:56:LEU:N	2.48	0.47
1:C:234:THR:HA	1:C:237:GLU:CB	2.45	0.47
1:C:592:ILE:C	1:C:594:LYS:N	2.67	0.47
1:D:53:THR:HA	1:D:56:LEU:CB	2.45	0.47
1:B:67:MET:C	1:B:69:THR:N	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:THR:HA	1:C:56:LEU:CB	2.44	0.47
1:C:265:THR:O	1:C:266:ASN:CB	2.62	0.47
1:A:300:TYR:HA	1:A:331:ALA:O	2.14	0.47
1:B:257:SER:CB	1:B:306:ALA:HB3	2.45	0.47
1:D:505:ILE:O	1:D:601:LEU:O	2.33	0.47
1:A:65:ALA:C	1:A:67:MET:N	2.73	0.46
1:A:486:ASP:C	1:A:488:ASN:H	2.23	0.46
1:B:301:LEU:O	1:B:333:TRP:N	2.47	0.46
1:C:551:ALA:HB2	1:C:597:VAL:C	2.40	0.46
1:B:303:PRO:C	1:B:305:HIS:H	2.24	0.46
1:A:197:TYR:HA	1:A:452:ALA:HB1	1.97	0.46
1:A:279:PHE:O	1:A:283:ALA:N	2.46	0.46
1:B:39:VAL:O	1:B:42:ARG:N	2.49	0.46
1:C:522:PRO:O	1:C:528:ALA:HB1	2.15	0.46
1:A:64:CYS:CB	1:A:78:ALA:HB2	2.46	0.46
1:A:349:THR:HA	1:A:382:THR:HA	1.98	0.46
1:C:730:TYR:C	1:C:732:TRP:H	2.23	0.46
1:B:287:ASP:HA	1:B:294:PRO:CA	2.45	0.46
1:A:273:ILE:C	1:A:275:MET:N	2.75	0.45
1:A:474:ALA:HB3	1:A:542:ALA:HB1	1.98	0.45
1:B:213:PRO:O	1:B:489:TYR:N	2.49	0.45
1:D:471:HIS:HA	1:D:542:ALA:HB2	1.98	0.45
1:B:404:VAL:O	1:B:739:GLY:N	2.49	0.45
1:B:572:PHE:N	1:B:704:VAL:O	2.49	0.45
1:B:445:LEU:O	1:B:446:ALA:HB2	2.17	0.45
1:A:5:LYS:C	1:A:7:ASP:H	2.24	0.45
1:B:280:ASN:C	1:B:282:THR:H	2.25	0.45
1:B:371:TYR:C	1:B:373:ARG:H	2.25	0.45
1:C:181:ARG:O	1:C:183:ILE:N	2.49	0.45
1:B:75:ALA:C	1:B:77:LEU:N	2.74	0.45
1:A:65:ALA:O	1:A:67:MET:N	2.50	0.45
1:C:592:ILE:HA	1:C:596:GLY:H	1.82	0.45
1:A:104:TYR:O	1:A:113:ALA:N	2.34	0.44
1:A:119:ASP:C	1:A:121:TYR:N	2.74	0.44
1:B:83:ILE:C	1:B:85:ASN:H	2.25	0.44
1:C:174:VAL:HA	1:C:208:ALA:CB	2.47	0.44
1:A:513:ALA:HB3	1:A:618:ASN:CB	2.47	0.44
1:D:249:GLY:HA2	1:D:298:ALA:H	1.81	0.44
1:A:59:LEU:O	1:A:63:THR:N	2.50	0.44
1:B:212:LYS:O	1:B:214:GLN:N	2.50	0.44
1:A:425:SER:HA	1:A:431:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:ARG:HA	1:C:746:GLN:C	2.43	0.44
1:D:457:SER:O	1:D:459:ASP:N	2.48	0.44
1:A:148:PHE:C	1:A:150:THR:H	2.25	0.44
1:A:486:ASP:O	1:A:488:ASN:N	2.51	0.44
1:B:335:PRO:C	1:B:337:LEU:N	2.76	0.44
1:A:148:PHE:C	1:A:150:THR:N	2.75	0.43
1:C:539:ILE:C	1:C:541:HIS:H	2.26	0.43
1:A:277:ARG:HA	1:A:280:ASN:CB	2.48	0.43
1:D:538:THR:O	1:D:542:ALA:N	2.52	0.43
1:A:287:ASP:O	1:A:290:GLY:N	2.52	0.43
1:B:62:GLU:O	1:B:65:ALA:HB3	2.18	0.43
1:B:273:ILE:C	1:B:275:MET:H	2.25	0.43
1:B:526:GLU:C	1:B:528:ALA:H	2.25	0.43
1:A:299:LEU:N	1:A:329:PHE:O	2.51	0.43
1:A:506:ALA:CB	1:A:604:ALA:HB3	2.49	0.43
1:A:516:PHE:C	1:A:518:LEU:H	2.27	0.43
1:A:493:GLU:O	1:A:497:LYS:N	2.49	0.43
1:C:516:PHE:C	1:C:518:LEU:H	2.27	0.43
1:D:545:GLU:C	1:D:547:SER:H	2.26	0.43
1:B:407:LYS:C	1:B:409:ALA:N	2.76	0.43
1:D:486:ASP:C	1:D:488:ASN:H	2.27	0.43
1:B:86:LEU:C	1:B:88:LYS:N	2.77	0.43
1:C:59:LEU:O	1:C:63:THR:N	2.51	0.43
1:C:563:SER:O	1:C:565:ALA:N	2.52	0.43
1:D:585:TRP:C	1:D:587:THR:H	2.27	0.42
1:C:195:LEU:C	1:C:197:TYR:H	2.26	0.42
1:D:191:ASN:C	1:D:193:MET:H	2.25	0.42
1:A:37:VAL:C	1:A:39:VAL:H	2.28	0.42
1:C:703:SER:HA	1:C:706:ILE:CB	2.49	0.42
1:D:68:THR:C	1:D:70:VAL:H	2.28	0.42
1:A:22:ILE:O	1:A:26:CYS:N	2.53	0.42
1:B:694:THR:C	1:B:696:ILE:N	2.78	0.42
1:D:389:TRP:C	1:D:391:SER:H	2.27	0.42
1:B:65:ALA:C	1:B:67:MET:N	2.76	0.42
1:B:565:ALA:HA	1:B:569:ILE:O	2.19	0.42
1:C:79:ALA:HA	1:C:82:ALA:HB3	2.01	0.42
1:C:475:LYS:HA	1:C:546:ALA:HB2	2.01	0.42
1:D:406:TYR:CB	1:D:409:ALA:HB3	2.49	0.42
1:C:483:ARG:HA	1:C:486:ASP:CB	2.49	0.42
1:B:147:GLY:HA2	1:B:614:ILE:HA	2.01	0.42
1:C:207:ASN:O	1:C:208:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:O	1:A:289:GLY:N	2.52	0.41
1:B:283:ALA:HB1	1:B:295:GLY:O	2.19	0.41
1:B:627:ASN:O	1:B:641:VAL:HA	2.20	0.41
1:C:699:ALA:C	1:C:701:ASP:H	2.28	0.41
1:B:626:SER:C	1:B:628:MET:N	2.79	0.41
1:C:642:ASN:CB	1:C:645:LEU:CB	2.98	0.41
1:B:39:VAL:O	1:B:40:THR:C	2.63	0.41
1:A:159:ILE:C	1:A:161:GLY:H	2.28	0.41
1:B:516:PHE:C	1:B:518:LEU:N	2.78	0.41
1:D:231:ILE:O	1:D:235:LEU:N	2.54	0.41
1:D:475:LYS:HA	1:D:546:ALA:HB2	2.02	0.41
1:A:287:ASP:O	1:A:289:GLY:N	2.53	0.41
1:B:663:LEU:C	1:B:665:THR:H	2.27	0.41
1:D:248:ILE:O	1:D:297:PHE:HA	2.20	0.41
1:A:27:TYR:C	1:A:29:LEU:N	2.70	0.41
1:B:391:SER:HA	1:B:394:GLU:CB	2.50	0.41
1:D:513:ALA:O	1:D:514:ASP:C	2.63	0.41
1:A:76:THR:HA	1:A:79:ALA:HB3	2.02	0.40
1:B:204:THR:O	1:B:208:ALA:HB2	2.21	0.40
1:B:629:TYR:O	1:B:630:SER:C	2.64	0.40
1:B:405:VAL:HA	1:B:738:THR:HA	2.03	0.40
1:B:473:ILE:C	1:B:475:LYS:H	2.29	0.40
1:B:680:LEU:HA	1:B:683:LEU:CB	2.51	0.40
1:D:304:TRP:O	1:D:351:PHE:N	2.55	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	735/888 (83%)	533 (72%)	157 (21%)	45 (6%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	735/888 (83%)	518 (70%)	180 (24%)	37 (5%)	1	16
1	C	735/888 (83%)	536 (73%)	154 (21%)	45 (6%)	1	13
1	D	735/888 (83%)	542 (74%)	148 (20%)	45 (6%)	1	13
All	All	2940/3552 (83%)	2129 (72%)	639 (22%)	172 (6%)	1	13

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	GLU
1	A	227	SER
1	A	288	GLN
1	A	461	LYS
1	A	486	ASP
1	A	677	PRO
1	B	501	ARG
1	B	719	PRO
1	C	5	LYS
1	C	145	TYR
1	C	291	ASN
1	C	318	HIS
1	C	320	LYS
1	D	5	LYS
1	D	196	LYS
1	D	227	SER
1	D	291	ASN
1	D	667	ASN
1	D	677	PRO
1	A	120	VAL
1	A	290	GLY
1	A	487	ARG
1	A	558	GLU
1	A	613	GLN
1	A	623	PRO
1	A	674	PRO
1	B	159	ILE
1	B	364	GLY
1	B	452	ALA
1	C	108	ALA
1	C	159	ILE
1	C	182	ASP
1	C	288	GLN

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Mol	Chain	Res	Type
1	C	319	GLY
1	C	364	GLY
1	C	491	PRO
1	C	706	ILE
1	D	159	ILE
1	D	206	PHE
1	D	288	GLN
1	D	318	HIS
1	D	319	GLY
1	D	343	GLU
1	D	344	GLU
1	D	522	PRO
1	D	719	PRO
1	A	6	ARG
1	A	8	GLY
1	A	66	TYR
1	A	201	ALA
1	A	259	GLY
1	A	353	PRO
1	A	501	ARG
1	A	679	GLU
1	A	708	GLN
1	A	741	TYR
1	B	50	GLY
1	B	87	HIS
1	B	109	THR
1	B	175	ALA
1	B	264	GLY
1	B	345	ASN
1	B	437	PRO
1	B	626	SER
1	B	740	MET
1	B	745	THR
1	C	4	TYR
1	C	12	PRO
1	C	160	ASN
1	C	266	ASN
1	C	273	ILE
1	C	322	GLU
1	C	426	ASN
1	C	522	PRO
1	C	532	ASN

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Mol	Chain	Res	Type
1	C	581	GLY
1	C	606	MET
1	D	145	TYR
1	D	257	SER
1	D	266	ASN
1	D	345	ASN
1	D	462	THR
1	D	609	ALA
1	D	686	THR
1	A	153	ARG
1	A	159	ILE
1	A	304	TRP
1	A	318	HIS
1	A	492	VAL
1	A	608	THR
1	A	657	GLU
1	B	8	GLY
1	B	12	PRO
1	B	191	ASN
1	B	266	ASN
1	B	304	TRP
1	B	458	GLU
1	B	580	TYR
1	B	656	ASP
1	B	737	LYS
1	C	76	THR
1	C	155	TYR
1	C	211	PRO
1	C	345	ASN
1	C	558	GLU
1	C	564	PRO
1	C	567	GLN
1	C	719	PRO
1	C	745	THR
1	D	50	GLY
1	D	119	ASP
1	D	259	GLY
1	D	264	GLY
1	D	458	GLU
1	D	493	GLU
1	D	582	MET
1	D	586	ASP

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Mol	Chain	Res	Type
1	D	662	TYR
1	D	741	TYR
1	A	110	GLY
1	A	160	ASN
1	A	345	ASN
1	A	460	GLY
1	A	571	GLN
1	B	93	GLN
1	B	210	THR
1	B	273	ILE
1	B	387	LYS
1	B	459	ASP
1	B	558	GLU
1	B	617	TYR
1	B	620	CYS
1	B	661	GLN
1	C	18	ILE
1	C	257	SER
1	C	264	GLY
1	C	351	PHE
1	C	538	THR
1	C	580	TYR
1	C	642	ASN
1	D	292	LYS
1	D	353	PRO
1	D	579	PRO
1	D	737	LYS
1	A	266	ASN
1	A	417	LYS
1	A	511	GLY
1	C	51	VAL
1	D	114	PRO
1	D	153	ARG
1	D	374	TYR
1	D	684	TYR
1	A	28	GLY
1	A	274	PRO
1	C	50	GLY
1	A	564	PRO
1	B	31	PRO
1	B	180	GLY
1	B	213	PRO

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Mol	Chain	Res	Type
1	C	676	VAL
1	D	203	PRO
1	D	511	GLY
1	A	30	ASP
1	A	241	ILE
1	A	276	ILE
1	B	454	ILE
1	C	677	PRO
1	D	491	PRO
1	D	623	PRO
1	D	690	ILE
1	A	163	VAL
1	C	178	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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 ⓘ

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	739/888 (83%)	-0.08	29 (3%) 43 42	39, 81, 170, 183	0
1	B	739/888 (83%)	-0.10	27 (3%) 45 43	52, 74, 175, 188	0
1	C	739/888 (83%)	-0.07	26 (3%) 47 43	51, 73, 173, 194	0
1	D	739/888 (83%)	-0.11	29 (3%) 43 42	58, 80, 175, 186	0
All	All	2956/3552 (83%)	-0.09	111 (3%) 44 42	39, 78, 173, 194	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	691	SER	8.2
1	A	522	PRO	7.5
1	B	562	GLY	7.4
1	B	746	GLN	6.5
1	D	90	THR	5.9
1	A	674	PRO	5.6
1	C	561	GLN	5.4
1	D	166	ARG	5.2
1	A	558	GLU	5.1
1	C	215	MET	4.7
1	A	127	ASN	4.6
1	A	329	PHE	4.5
1	B	30	ASP	4.3
1	A	709	SER	4.3
1	C	384	LYS	4.1
1	A	128	LYS	4.1
1	C	380	GLY	4.0
1	D	547	SER	3.9
1	B	147	GLY	3.9
1	C	578	LYS	3.9
1	B	613	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	713	ASN	3.7
1	D	321	GLU	3.7
1	B	386	GLN	3.7
1	D	573	ASP	3.7
1	B	104	TYR	3.5
1	D	580	TYR	3.5
1	B	415	ASN	3.5
1	C	568	GLY	3.5
1	B	385	ALA	3.5
1	C	214	GLN	3.5
1	B	8	GLY	3.4
1	A	577	GLN	3.4
1	A	692	GLN	3.4
1	A	443	CYS	3.2
1	B	102	TYR	3.2
1	B	709	SER	3.2
1	A	714	LEU	3.2
1	D	601	LEU	3.2
1	D	322	GLU	3.2
1	C	71	HIS	3.2
1	B	570	LEU	3.1
1	C	597	VAL	3.1
1	C	157	LEU	3.1
1	A	330	PRO	3.1
1	B	739	GLY	3.0
1	B	573	ASP	3.0
1	D	323	ILE	3.0
1	C	579	PRO	3.0
1	B	184	GLU	2.9
1	D	45	SER	2.8
1	C	492	VAL	2.8
1	D	568	GLY	2.8
1	B	229	GLU	2.8
1	A	621	PHE	2.8
1	D	745	THR	2.8
1	C	415	ASN	2.7
1	D	609	ALA	2.7
1	B	136	VAL	2.7
1	D	518	LEU	2.7
1	A	16	ASP	2.6
1	C	385	ALA	2.6
1	A	715	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	443	CYS	2.6
1	A	233	ASP	2.6
1	A	435	SER	2.6
1	D	458	GLU	2.6
1	A	255	ILE	2.6
1	B	707	ASP	2.6
1	D	638	PHE	2.6
1	D	642	ASN	2.5
1	C	129	ASP	2.5
1	B	430	GLU	2.5
1	B	612	SER	2.5
1	B	135	ILE	2.4
1	D	413	LYS	2.4
1	D	444	ASN	2.4
1	A	622	GLU	2.4
1	D	493	GLU	2.4
1	C	345	ASN	2.4
1	A	166	ARG	2.4
1	C	162	GLN	2.3
1	D	661	GLN	2.3
1	A	444	ASN	2.3
1	D	182	ASP	2.3
1	A	317	ASN	2.3
1	C	223	MET	2.3
1	C	507	LEU	2.2
1	C	73	ASP	2.2
1	C	715	PHE	2.2
1	A	306	ALA	2.2
1	B	480	ASN	2.2
1	C	79	ALA	2.2
1	D	454	ILE	2.2
1	B	433	GLU	2.2
1	C	284	ARG	2.2
1	A	491	PRO	2.1
1	B	316	LYS	2.1
1	D	627	ASN	2.1
1	D	545	GLU	2.1
1	D	613	GLN	2.1
1	D	644	TYR	2.1
1	C	217	SER	2.1
1	D	586	ASP	2.1
1	A	91	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	204	THR	2.0
1	A	430	GLU	2.0
1	A	711	SER	2.0
1	A	328	LEU	2.0
1	D	739	GLY	2.0
1	C	740	MET	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.