



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 AM UTC

PDB ID : 7MI1 / pdb_00007mi1
Title : X-ray structure of yeast dynein motor domain in the presence of a pyrazolo-pyrimidinone-based compound (compound 20)
Authors : Santarossa, C.C.; Ekiert, D.C.; Bhabha, G.; Kapoor, T.M.
Deposited on : 2021-04-16
Resolution : 4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

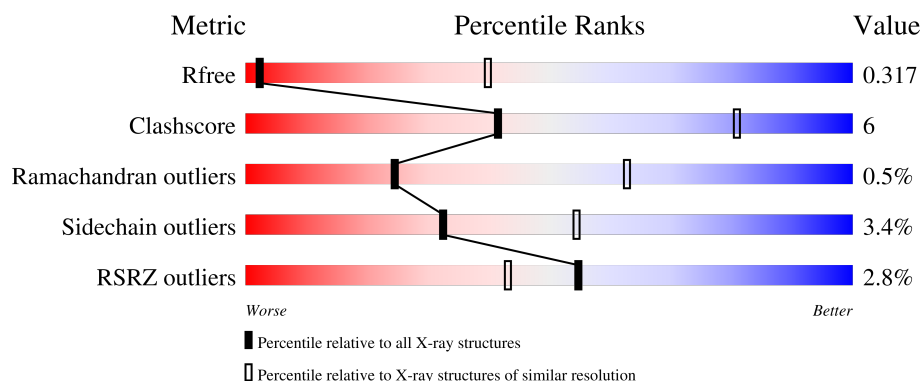
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	2661	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 42528 atoms, of which 21316 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 Chimera protein of Dynein and Endolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	2628	42528	13593	21316	3538	3984	97	0	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1363	GLY	-	expression tag	UNP P36022
A	1849	GLN	GLU	engineered mutation	UNP P36022
A	3120	GLY	-	linker	UNP P36022
A	3121	SER	-	linker	UNP P36022
A	3122	GLY	-	linker	UNP P36022
A	3123	SER	-	linker	UNP P36022
A	3124	GLY	-	linker	UNP P36022
A	3125	SER	-	linker	UNP P36022
A	3178	THR	CYS	conflict	UNP D9IEF7
A	3221	ALA	CYS	conflict	UNP D9IEF7
A	3286	GLY	-	linker	UNP D9IEF7
A	3287	SER	-	linker	UNP D9IEF7
A	3288	GLY	-	linker	UNP D9IEF7
A	3289	SER	-	linker	UNP D9IEF7
A	3290	GLY	-	linker	UNP D9IEF7
A	3291	SER	-	linker	UNP D9IEF7
A	3742	ASP	ASN	conflict	UNP P36022
A	3895	VAL	PHE	conflict	UNP P36022
A	4072	ASP	ASN	conflict	UNP P36022
A	4093	GLY	-	expression tag	UNP P36022
A	4094	SER	-	expression tag	UNP P36022
A	4095	GLY	-	expression tag	UNP P36022
A	4096	SER	-	expression tag	UNP P36022
A	4097	GLY	-	expression tag	UNP P36022
A	4098	SER	-	expression tag	UNP P36022
A	4099	HIS	-	expression tag	UNP P36022
A	4100	HIS	-	expression tag	UNP P36022

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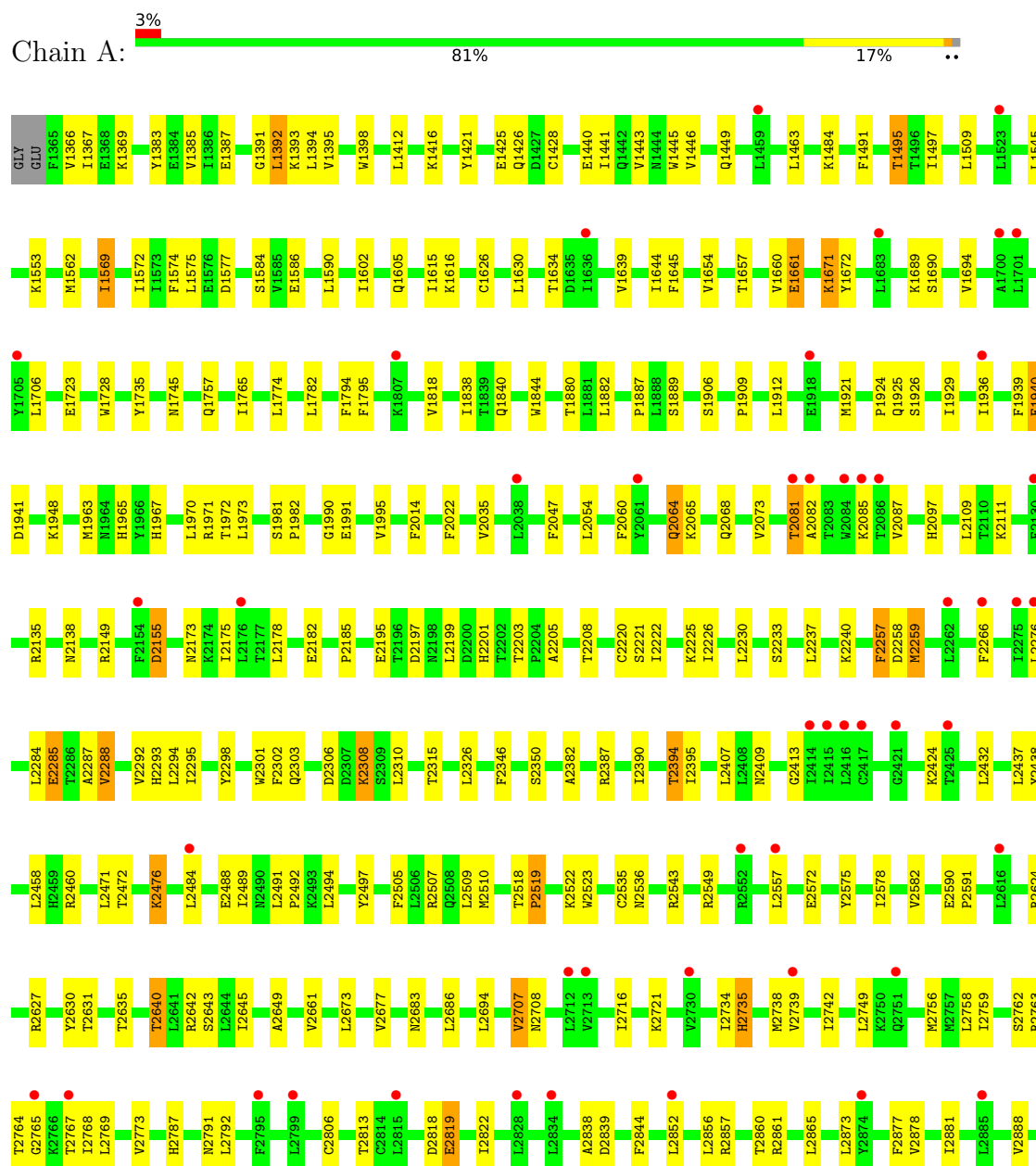
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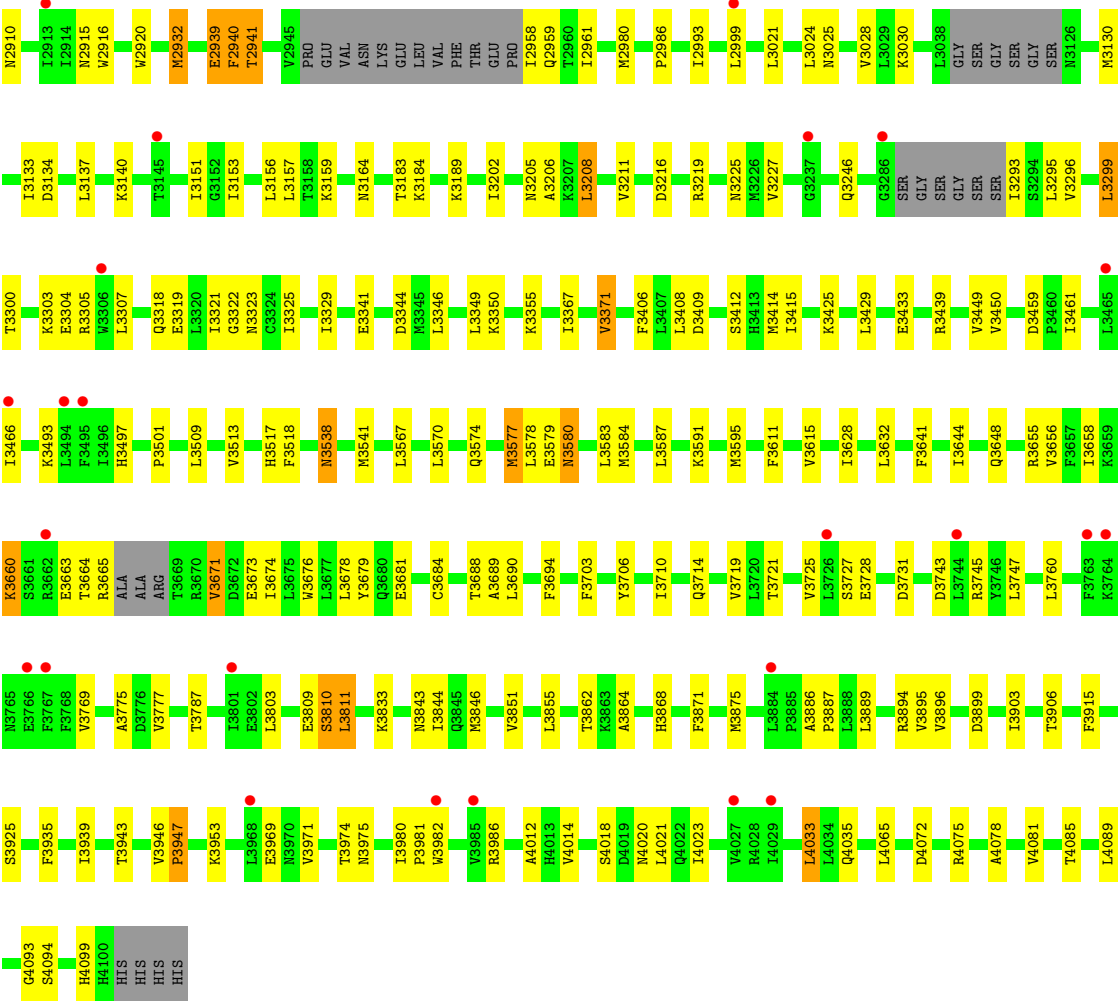
Chain	Residue	Modelled	Actual	Comment	Reference
A	4101	HIS	-	expression tag	UNP P36022
A	4102	HIS	-	expression tag	UNP P36022
A	4103	HIS	-	expression tag	UNP P36022
A	4104	HIS	-	expression tag	UNP P36022

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: Chimera protein of Dynein and Endolysin





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	135.06Å 157.92Å 179.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 4.50 47.66 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.66-4.50) 99.4 (47.66-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.276 , 0.320 0.276 , 0.317	Depositor DCC
R_{free} test set	2000 reflections (8.58%)	wwPDB-VP
Wilson B-factor (Å ²)	183.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 168.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	42528	wwPDB-VP
Average B, all atoms (Å ²)	228.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 [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	0.14	0/21632	0.34	4/29225 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2941	THR	N-CA-C	6.65	124.97	110.80
1	A	2940	PHE	N-CA-C	5.77	123.09	110.80
1	A	2940	PHE	CA-C-N	5.50	132.05	121.54
1	A	2940	PHE	C-N-CA	5.50	132.05	121.54

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	21212	21316	21315	271	0
All	All	21212	21316	21315	271	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 6.

All (271) 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:3665:ARG:NH1	1:A:3673:GLU:OE2	1.97	0.97
1:A:2939:GLU:OE1	1:A:3318:GLN:NE2	2.05	0.89
1:A:2624:ARG:NH2	1:A:2910:ASN:O	2.08	0.86
1:A:2064:GLN:OE1	1:A:2065:LYS:N	2.15	0.79
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.64	0.77
1:A:1939:PHE:O	1:A:1941:ASP:N	2.19	0.75
1:A:3660:LYS:O	1:A:3660:LYS:NZ	2.21	0.74
1:A:2458:LEU:HD11	1:A:2484:LEU:HD11	1.69	0.73
1:A:1412:LEU:HD22	1:A:1428:CYS:SG	2.29	0.73
1:A:2155:ASP:OD2	1:A:2507:ARG:NH2	2.22	0.73
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.69	0.73
1:A:2135:ARG:NH2	1:A:2182:GLU:OE1	2.22	0.73
1:A:2877:PHE:CZ	1:A:2881:ILE:HD11	2.28	0.69
1:A:3946:VAL:HG11	1:A:3953:LYS:HB2	1.74	0.69
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.25	0.69
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.76	0.67
1:A:3809:GLU:O	1:A:3811:LEU:N	2.28	0.67
1:A:1967:HIS:O	1:A:1972:THR:OG1	2.07	0.67
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.77	0.67
1:A:2460:ARG:NH2	1:A:2839:ASP:OD2	2.28	0.66
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.78	0.65
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	1.79	0.64
1:A:2258:ASP:O	1:A:2259:MET:HB2	1.96	0.64
1:A:4072:ASP:OD1	1:A:4075:ARG:NH2	2.31	0.64
1:A:2220:CYS:SG	1:A:2221:SER:N	2.71	0.64
1:A:3466:ILE:HD13	1:A:3509:LEU:CD1	2.29	0.63
1:A:2060:PHE:HD2	1:A:2087:VAL:HG11	1.62	0.62
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.80	0.62
1:A:3307:LEU:HD12	1:A:3307:LEU:O	1.99	0.62
1:A:3130:MET:HE2	1:A:3225:ASN:HD22	1.66	0.61
1:A:2081:THR:HG22	1:A:2085:LYS:HE3	1.84	0.60
1:A:3296:VAL:HA	1:A:3584:MET:SD	2.42	0.60
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.17	0.60
1:A:2258:ASP:O	1:A:2259:MET:CB	2.50	0.59
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.85	0.59
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.38	0.59
1:A:2631:THR:O	1:A:2635:THR:HG22	2.04	0.58
1:A:2806:CYS:HG	1:A:2813:THR:HG1	1.45	0.58
1:A:2138:ASN:ND2	1:A:2185:PRO:O	2.37	0.57
1:A:2230:LEU:HD11	1:A:2257:PHE:HZ	1.69	0.57
1:A:3028:VAL:HG12	1:A:3300:THR:HB	1.86	0.57
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3843:ASN:HB3	1:A:3846:MET:HE3	1.87	0.57
1:A:1425:GLU:O	1:A:1428:CYS:N	2.37	0.56
1:A:1929:ILE:HD13	1:A:1970:LEU:HD11	1.87	0.56
1:A:3346:LEU:HD11	1:A:3350:LYS:HE3	1.87	0.56
1:A:1774:LEU:HD21	1:A:1921:MET:HE1	1.87	0.56
1:A:1706:LEU:HD12	1:A:1936:ILE:HD13	1.86	0.56
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.36	0.56
1:A:1661:GLU:OE2	1:A:1735:TYR:OH	2.22	0.56
1:A:2582:VAL:HG23	1:A:2582:VAL:O	2.06	0.56
1:A:1745:ASN:OD1	1:A:1757:GLN:NE2	2.40	0.56
1:A:1940:GLU:OE1	1:A:1990:GLY:HA2	2.06	0.56
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.88	0.55
1:A:2458:LEU:HD21	1:A:2484:LEU:HD21	1.89	0.55
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.89	0.54
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.88	0.54
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.71	0.54
1:A:2818:ASP:OD1	1:A:2819:GLU:N	2.41	0.54
1:A:2197:ASP:N	1:A:2197:ASP:OD1	2.39	0.54
1:A:1991:GLU:O	1:A:1995:VAL:HG23	2.07	0.54
1:A:1925:GLN:O	1:A:1929:ILE:HD12	2.08	0.54
1:A:2413:GLY:HA3	1:A:2510:MET:HE3	1.89	0.54
1:A:2522:LYS:HG2	1:A:2523:TRP:H	1.73	0.54
1:A:3211:VAL:HG22	1:A:3246:GLN:HB3	1.90	0.53
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.73	0.53
1:A:2762:SER:O	1:A:2764:THR:N	2.42	0.53
1:A:2394:THR:HG22	1:A:2395:ILE:HD12	1.90	0.53
1:A:3971:VAL:HA	1:A:3974:THR:HG22	1.90	0.53
1:A:1366:VAL:HG13	1:A:1369:LYS:HE3	1.91	0.53
1:A:2762:SER:C	1:A:2764:THR:H	2.17	0.52
1:A:1838:ILE:HD11	1:A:1844:TRP:C	2.34	0.52
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.90	0.52
1:A:3678:LEU:HD23	1:A:3678:LEU:C	2.34	0.52
1:A:1971:ARG:HB2	1:A:2208:THR:HG21	1.90	0.52
1:A:2932:MET:HE1	1:A:2993:ILE:HG23	1.92	0.52
1:A:2407:LEU:HD12	1:A:2557:LEU:HD11	1.92	0.52
1:A:1395:VAL:HG23	1:A:1398:TRP:NE1	2.25	0.51
1:A:2471:LEU:HD12	1:A:2471:LEU:H	1.76	0.51
1:A:3895:VAL:HG12	1:A:3896:VAL:N	2.26	0.51
1:A:3134:ASP:OD2	1:A:3225:ASN:ND2	2.41	0.51
1:A:3980:ILE:N	1:A:3981:PRO:CD	2.73	0.51
1:A:3775:ALA:HB2	1:A:3803:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:ILE:H	1:A:1367:ILE:HD12	1.76	0.51
1:A:3216:ASP:OD2	1:A:3219:ARG:NH1	2.43	0.51
1:A:3703:PHE:HE2	1:A:3719:VAL:HG21	1.75	0.51
1:A:1840:GLN:OE1	1:A:1887:PRO:HG2	2.11	0.51
1:A:2940:PHE:CB	1:A:3318:GLN:OE1	2.58	0.51
1:A:2073:VAL:HG21	1:A:2199:LEU:HD11	1.93	0.50
1:A:3322:GLY:HA2	1:A:3325:ILE:HD12	1.93	0.50
1:A:3433:GLU:OE2	1:A:3439:ARG:NH2	2.44	0.50
1:A:3663:GLU:C	1:A:3665:ARG:H	2.19	0.50
1:A:1909:PRO:HD2	1:A:1912:LEU:HD12	1.93	0.50
1:A:3329:ILE:HG21	1:A:3349:LEU:HD22	1.92	0.50
1:A:3299:LEU:HD11	1:A:3587:LEU:CB	2.40	0.50
1:A:2315:THR:HG21	1:A:2350:SER:HB3	1.94	0.50
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.94	0.50
1:A:1939:PHE:O	1:A:1940:GLU:C	2.54	0.50
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.94	0.50
1:A:1671:LYS:HD3	1:A:1672:TYR:N	2.26	0.49
1:A:3202:ILE:HD11	1:A:3227:VAL:HG21	1.93	0.49
1:A:3367:ILE:O	1:A:3371:VAL:HG22	2.12	0.49
1:A:2294:LEU:O	1:A:2298:TYR:CD2	2.66	0.49
1:A:2522:LYS:HG2	1:A:2523:TRP:N	2.28	0.49
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.94	0.49
1:A:3304:GLU:O	1:A:3307:LEU:HD23	2.13	0.49
1:A:3925:SER:OG	1:A:3969:GLU:OE2	2.29	0.49
1:A:2306:ASP:O	1:A:2310:LEU:HB2	2.12	0.49
1:A:2980:MET:HE1	1:A:3341:GLU:HB3	1.94	0.49
1:A:3293:ILE:O	1:A:3296:VAL:HG12	2.12	0.49
1:A:2237:LEU:O	1:A:2240:LYS:O	2.31	0.49
1:A:1630:LEU:HD23	1:A:1634:THR:CG2	2.43	0.49
1:A:3684:CYS:HB2	1:A:3769:VAL:HG11	1.95	0.49
1:A:3412:SER:O	1:A:3415:ILE:HG22	2.12	0.48
1:A:4014:VAL:O	1:A:4021:LEU:HD21	2.13	0.48
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	1.96	0.48
1:A:1445:TRP:HB2	1:A:1509:LEU:HD13	1.96	0.48
1:A:3429:LEU:HD13	1:A:3450:VAL:HG13	1.94	0.48
1:A:3706:TYR:CZ	1:A:3710:ILE:CD1	2.96	0.48
1:A:3307:LEU:HD12	1:A:3307:LEU:C	2.37	0.48
1:A:3760:LEU:HD21	1:A:4078:ALA:HA	1.95	0.48
1:A:2109:LEU:HD22	1:A:2518:THR:HG22	1.95	0.48
1:A:3570:LEU:HD21	1:A:3583:LEU:HD21	1.95	0.48
1:A:3580:ASN:O	1:A:3584:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3648:GLN:OE1	1:A:3894:ARG:NH2	2.46	0.48
1:A:1562:MET:HB2	1:A:1569:ILE:HD11	1.95	0.48
1:A:3299:LEU:HD11	1:A:3587:LEU:HB3	1.95	0.48
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.96	0.48
1:A:2233:SER:HB3	1:A:2292:VAL:HG11	1.96	0.47
1:A:2394:THR:HG22	1:A:2395:ILE:H	1.78	0.47
1:A:2791:ASN:OD1	1:A:2792:LEU:N	2.48	0.47
1:A:3580:ASN:OD1	1:A:3580:ASN:N	2.46	0.47
1:A:2035:VAL:HG23	1:A:2054:LEU:HD11	1.97	0.47
1:A:2940:PHE:HB2	1:A:3318:GLN:OE1	2.15	0.47
1:A:3449:VAL:HG13	1:A:3493:LYS:HB2	1.96	0.47
1:A:1416:LYS:HA	1:A:1421:TYR:CE1	2.50	0.47
1:A:3408:LEU:HD21	1:A:3501:PRO:HG3	1.96	0.47
1:A:3414:MET:HE3	1:A:3518:PHE:CD1	2.49	0.47
1:A:3658:ILE:HD12	1:A:3658:ILE:N	2.30	0.47
1:A:3024:LEU:HD11	1:A:3303:LYS:HE2	1.97	0.47
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.96	0.47
1:A:3133:ILE:HD11	1:A:3295:LEU:HD11	1.96	0.47
1:A:3151:ILE:HB	1:A:3157:LEU:HD11	1.96	0.47
1:A:3321:ILE:HD12	1:A:3321:ILE:H	1.79	0.47
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.97	0.46
1:A:1630:LEU:HA	1:A:1634:THR:HG22	1.97	0.46
1:A:1366:VAL:HG12	1:A:1366:VAL:O	2.15	0.46
1:A:3030:LYS:NZ	1:A:3574:GLN:OE1	2.48	0.46
1:A:2640:THR:HG23	1:A:2643:SER:H	1.81	0.46
1:A:1590:LEU:HD13	1:A:1644:ILE:HD13	1.97	0.46
1:A:1782:LEU:HD21	1:A:1794:PHE:CZ	2.50	0.46
1:A:2518:THR:OG1	1:A:2519:PRO:HD3	2.15	0.46
1:A:3587:LEU:O	1:A:3591:LYS:HG2	2.14	0.46
1:A:2195:GLU:OE2	1:A:2549:ARG:NH2	2.49	0.46
1:A:2734:ILE:H	1:A:2734:ILE:HD12	1.81	0.46
1:A:2432:LEU:HD22	1:A:2438:TYR:HB2	1.98	0.46
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.98	0.46
1:A:3183:THR:OG1	1:A:3184:LYS:N	2.50	0.45
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.97	0.45
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.82	0.45
1:A:3024:LEU:O	1:A:3028:VAL:HG13	2.16	0.45
1:A:1385:VAL:HG21	1:A:1491:PHE:CD1	2.51	0.45
1:A:1392:LEU:HD23	1:A:1484:LYS:HG2	1.99	0.45
1:A:3021:LEU:HA	1:A:3024:LEU:HD12	1.99	0.45
1:A:3025:ASN:O	1:A:3028:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3656:VAL:HG22	1:A:3681:GLU:HG3	1.99	0.45
1:A:3864:ALA:O	1:A:3868:HIS:N	2.49	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.98	0.44
1:A:2575:TYR:HA	1:A:2578:ILE:HG12	1.99	0.44
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.99	0.44
1:A:3688:THR:HG21	1:A:3777:VAL:HG21	1.99	0.44
1:A:2060:PHE:CD2	1:A:2087:VAL:HG11	2.48	0.44
1:A:3137:LEU:HD13	1:A:3153:ILE:HG13	1.99	0.44
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.32	0.44
1:A:3689:ALA:C	1:A:3690:LEU:HD12	2.42	0.44
1:A:4018:SER:C	1:A:4020:ASN:H	2.26	0.44
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.53	0.44
1:A:2742:ILE:HG23	1:A:2773:VAL:HG22	1.99	0.44
1:A:1882:LEU:HG	1:A:1882:LEU:O	2.17	0.44
1:A:2287:ALA:O	1:A:2288:VAL:C	2.60	0.44
1:A:3202:ILE:HG23	1:A:3208:LEU:HB2	1.99	0.44
1:A:3833:LYS:HZ2	1:A:3862:THR:HG21	1.82	0.44
1:A:2014:PHE:C	1:A:2014:PHE:CD1	2.96	0.44
1:A:2877:PHE:CE2	1:A:2881:ILE:HD11	2.53	0.44
1:A:3611:PHE:O	1:A:3615:VAL:HG13	2.18	0.43
1:A:3706:TYR:CE2	1:A:3710:ILE:HD12	2.53	0.43
1:A:1654:VAL:O	1:A:1657:THR:HG22	2.18	0.43
1:A:2308:LYS:HE3	1:A:2308:LYS:HA	2.00	0.43
1:A:3655:ARG:NH1	1:A:3681:GLU:OE1	2.51	0.43
1:A:1774:LEU:HD21	1:A:1921:MET:CE	2.48	0.43
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	2.00	0.43
1:A:3844:ILE:HD11	1:A:3855:LEU:HD22	1.99	0.43
1:A:3895:VAL:CG1	1:A:3896:VAL:N	2.82	0.43
1:A:1443:VAL:O	1:A:1446:VAL:HG12	2.18	0.43
1:A:2735:HIS:ND1	1:A:2738:MET:HB2	2.34	0.43
1:A:3809:GLU:O	1:A:3810:SER:C	2.61	0.43
1:A:2064:GLN:OE1	1:A:2064:GLN:C	2.62	0.43
1:A:2707:VAL:HG12	1:A:2708:ASN:H	1.83	0.43
1:A:3946:VAL:N	1:A:3947:PRO:CD	2.82	0.43
1:A:1572:ILE:HG23	1:A:1574:PHE:CE2	2.54	0.43
1:A:2627:ARG:O	1:A:2631:THR:HG23	2.18	0.43
1:A:2857:ARG:HG2	1:A:2861:ARG:HD3	2.00	0.43
1:A:3156:LEU:HD21	1:A:3159:LYS:HG3	2.00	0.43
1:A:1690:SER:HB3	1:A:1694:VAL:HG13	2.01	0.43
1:A:1929:ILE:HD12	1:A:1929:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3319:GLU:O	1:A:3323:ASN:ND2	2.37	0.42
1:A:3986:ARG:HD3	1:A:4012:ALA:HA	2.00	0.42
1:A:1545:LEU:C	1:A:1545:LEU:HD23	2.44	0.42
1:A:2756:MET:O	1:A:2888:VAL:HA	2.19	0.42
1:A:3409:ASP:OD1	1:A:3409:ASP:N	2.52	0.42
1:A:1689:LYS:O	1:A:1689:LYS:HG3	2.18	0.42
1:A:2222:ILE:HG22	1:A:2226:ILE:HD11	2.01	0.42
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.84	0.42
1:A:3408:LEU:HD23	1:A:3517:HIS:CE1	2.55	0.42
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.19	0.42
1:A:3851:VAL:HG13	1:A:3855:LEU:HB3	2.00	0.42
1:A:1425:GLU:O	1:A:1426:GLN:C	2.63	0.42
1:A:2109:LEU:CD2	1:A:2518:THR:HG22	2.49	0.42
1:A:2225:LYS:HD3	1:A:2284:LEU:HD12	2.01	0.42
1:A:2505:PHE:CE2	1:A:2509:LEU:HD11	2.54	0.42
1:A:2958:ILE:HG13	1:A:2959:GLN:H	1.85	0.42
1:A:3946:VAL:HG11	1:A:3953:LYS:CB	2.46	0.42
1:A:1394:LEU:HD22	1:A:1449:GLN:OE1	2.19	0.42
1:A:4021:LEU:HD23	1:A:4023:ILE:HG13	2.02	0.42
1:A:2759:ILE:O	1:A:2759:ILE:HG22	2.18	0.42
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.34	0.42
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.84	0.42
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.20	0.42
1:A:1660:VAL:HG11	1:A:1728:TRP:CH2	2.55	0.42
1:A:2382:ALA:HB1	1:A:2630:TYR:HE1	1.85	0.41
1:A:2649:ALA:HB1	1:A:2673:LEU:HD21	2.02	0.41
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	2.01	0.41
1:A:4085:THR:O	1:A:4089:LEU:HG	2.19	0.41
1:A:3743:ASP:OD1	1:A:3743:ASP:N	2.53	0.41
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	2.03	0.41
1:A:3409:ASP:OD1	1:A:3497:HIS:NE2	2.53	0.41
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.02	0.41
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.50	0.41
1:A:3903:ILE:HD12	1:A:3903:ILE:H	1.85	0.41
1:A:2572:GLU:HG3	1:A:2590:GLU:HA	2.03	0.41
1:A:2661:VAL:HG12	1:A:2916:TRP:CE2	2.56	0.41
1:A:2787:HIS:HB2	1:A:3459:ASP:HB2	2.01	0.41
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.61	0.41
1:A:1795:PHE:O	1:A:1795:PHE:CD1	2.74	0.41
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.85	0.41
1:A:2642:ARG:O	1:A:2645:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4081:VAL:O	1:A:4085:THR:HG23	2.20	0.41
1:A:4089:LEU:HB3	1:A:4094:SER:OG	2.20	0.41
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	2.03	0.41
1:A:1575:LEU:C	1:A:1577:ASP:H	2.29	0.41
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.56	0.41
1:A:2491:LEU:N	1:A:2492:PRO:CD	2.84	0.41
1:A:2590:GLU:N	1:A:2591:PRO:HD2	2.35	0.41
1:A:2856:LEU:HD21	1:A:2877:PHE:HB2	2.03	0.41
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.21	0.41
1:A:2765:GLY:CA	1:A:2768:ILE:HG22	2.51	0.41
1:A:3676:TRP:CD1	1:A:3706:TYR:CZ	3.09	0.41
1:A:1926:SER:HB2	1:A:1973:LEU:HD21	2.02	0.40
1:A:2097:HIS:HB2	1:A:2149:ARG:HE	1.86	0.40
1:A:4018:SER:O	1:A:4020:ASN:N	2.54	0.40
1:A:1963:MET:HG2	1:A:1965:HIS:CE1	2.57	0.40
1:A:2225:LYS:NZ	1:A:2285:GLU:OE2	2.35	0.40
1:A:2844:PHE:CG	1:A:2852:LEU:HD22	2.55	0.40
1:A:3727:SER:OG	1:A:3728:GLU:N	2.54	0.40
1:A:1615:ILE:HG13	1:A:1616:LYS:N	2.37	0.40
1:A:1948:LYS:NZ	1:A:1991:GLU:OE1	2.54	0.40
1:A:3577:MET:C	1:A:3579:GLU:H	2.27	0.40
1:A:2716:ILE:HD12	1:A:2739:VAL:HG22	2.02	0.40
1:A:3205:ASN:O	1:A:3206:ALA:HB3	2.21	0.40
1:A:3915:PHE:CD1	1:A:3915:PHE:C	2.99	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	2618/2661 (98%)	2464 (94%)	141 (5%)	13 (0%)	24 63

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1940	GLU
1	A	3810	SER
1	A	4099	HIS
1	A	1391	GLY
1	A	2259	MET
1	A	2763	ARG
1	A	2301	TRP
1	A	2519	PRO
1	A	3947	PRO
1	A	2986	PRO
1	A	3664	THR
1	A	4093	GLY
1	A	2288	VAL

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	2381/2406 (99%)	2299 (97%)	82 (3%)	32 54

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1383	TYR
1	A	1392	LEU
1	A	1440	GLU
1	A	1441	ILE
1	A	1463	LEU
1	A	1495	THR
1	A	1553	LYS
1	A	1569	ILE
1	A	1602	ILE
1	A	1605	GLN
1	A	1661	GLU
1	A	1671	LYS

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Mol	Chain	Res	Type
1	A	1723	GLU
1	A	1818	VAL
1	A	1880	THR
1	A	1889	SER
1	A	1906	SER
1	A	2064	GLN
1	A	2068	GLN
1	A	2081	THR
1	A	2111	LYS
1	A	2155	ASP
1	A	2257	PHE
1	A	2276	LEU
1	A	2285	GLU
1	A	2295	ILE
1	A	2302	PHE
1	A	2303	GLN
1	A	2308	LYS
1	A	2346	PHE
1	A	2394	THR
1	A	2424	LYS
1	A	2472	THR
1	A	2476	LYS
1	A	2494	LEU
1	A	2640	THR
1	A	2683	ASN
1	A	2694	LEU
1	A	2707	VAL
1	A	2721	LYS
1	A	2735	HIS
1	A	2767	THR
1	A	2769	LEU
1	A	2819	GLU
1	A	2822	ILE
1	A	2920	TRP
1	A	2932	MET
1	A	2939	GLU
1	A	2941	THR
1	A	2961	ILE
1	A	2999	LEU
1	A	3140	LYS
1	A	3164	ASN
1	A	3189	LYS

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Mol	Chain	Res	Type
1	A	3208	LEU
1	A	3299	LEU
1	A	3305	ARG
1	A	3344	ASP
1	A	3355	LYS
1	A	3371	VAL
1	A	3425	LYS
1	A	3538	ASN
1	A	3567	LEU
1	A	3577	MET
1	A	3578	LEU
1	A	3580	ASN
1	A	3595	MET
1	A	3660	LYS
1	A	3671	VAL
1	A	3714	GLN
1	A	3745	ARG
1	A	3747	LEU
1	A	3811	LEU
1	A	3871	PHE
1	A	3899	ASP
1	A	3906	THR
1	A	3939	ILE
1	A	3943	THR
1	A	3975	ASN
1	A	3982	TRP
1	A	4033	LEU
1	A	4065	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1707	HIS
1	A	1717	ASN
1	A	1870	ASN
1	A	1899	ASN
1	A	2228	HIS
1	A	2239	ASN
1	A	2430	ASN
1	A	3008	GLN
1	A	3401	GLN
1	A	3596	ASN

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Mol	Chain	Res	Type
1	A	3868	HIS
1	A	3878	HIS
1	A	3970	ASN
1	A	4099	HIS
1	A	4100	HIS

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 [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	2628/2661 (98%)	0.16	73 (2%) 55 43	159, 224, 285, 336	1 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2415	ILE	6.7
1	A	2799	LEU	5.9
1	A	2730	VAL	5.6
1	A	2084	TRP	5.6
1	A	1636	ILE	5.6
1	A	2416	LEU	4.5
1	A	2557	LEU	4.0
1	A	3766	GLU	3.8
1	A	1705	TYR	3.7
1	A	2086	THR	3.6
1	A	1936	ILE	3.6
1	A	2085	LYS	3.5
1	A	2885	LEU	3.5
1	A	1683	LEU	3.4
1	A	2176	LEU	3.4
1	A	2999	LEU	3.4
1	A	2874	TYR	3.4
1	A	2712	LEU	3.3
1	A	3145	THR	3.3
1	A	4027	VAL	3.2
1	A	2081	THR	3.2
1	A	4029	ILE	3.2
1	A	2739	VAL	3.1
1	A	3985	VAL	3.1
1	A	2828	LEU	3.1
1	A	2276	LEU	3.0
1	A	3465	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	3726	LEU	2.9
1	A	2130	PHE	2.9
1	A	2275	ILE	2.9
1	A	2061	TYR	2.9
1	A	2417	CYS	2.8
1	A	2767	THR	2.8
1	A	1701	LEU	2.7
1	A	3767	PHE	2.7
1	A	2852	LEU	2.6
1	A	2834	LEU	2.5
1	A	1700	ALA	2.5
1	A	3763	PHE	2.4
1	A	3286	GLY	2.4
1	A	2082	ALA	2.4
1	A	2266	PHE	2.4
1	A	3982	TRP	2.4
1	A	1523	LEU	2.4
1	A	3466	ILE	2.3
1	A	2616	LEU	2.3
1	A	3495	PHE	2.3
1	A	2262	LEU	2.2
1	A	2713	VAL	2.2
1	A	3662	ARG	2.2
1	A	3744	LEU	2.2
1	A	1918	GLU	2.2
1	A	2414	ILE	2.1
1	A	3764	LYS	2.1
1	A	2765	GLY	2.1
1	A	2425	THR	2.1
1	A	2552	ARG	2.1
1	A	2751	GLN	2.1
1	A	2913	ILE	2.1
1	A	2038	LEU	2.1
1	A	2421	GLY	2.1
1	A	1807	LYS	2.1
1	A	3237	GLY	2.1
1	A	2484	LEU	2.1
1	A	3801	ILE	2.1
1	A	2795	PHE	2.0
1	A	1459	LEU	2.0
1	A	2815	LEU	2.0
1	A	3884	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	3494	LEU	2.0
1	A	3968	LEU	2.0
1	A	2154	PHE	2.0
1	A	3306	TRP	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.