Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 10:37 PM EDT

PDB ID	:	7MI1
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 (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:

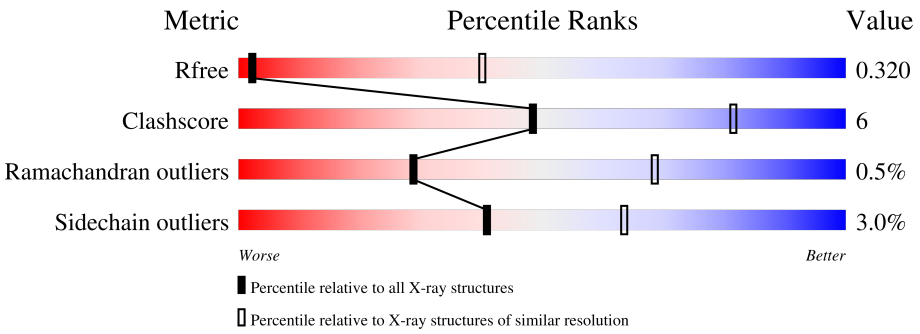
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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%

Mol	Chain	Length	Quality of chain
1	A	2661	81% 16% ••

2 Entry composition (i)

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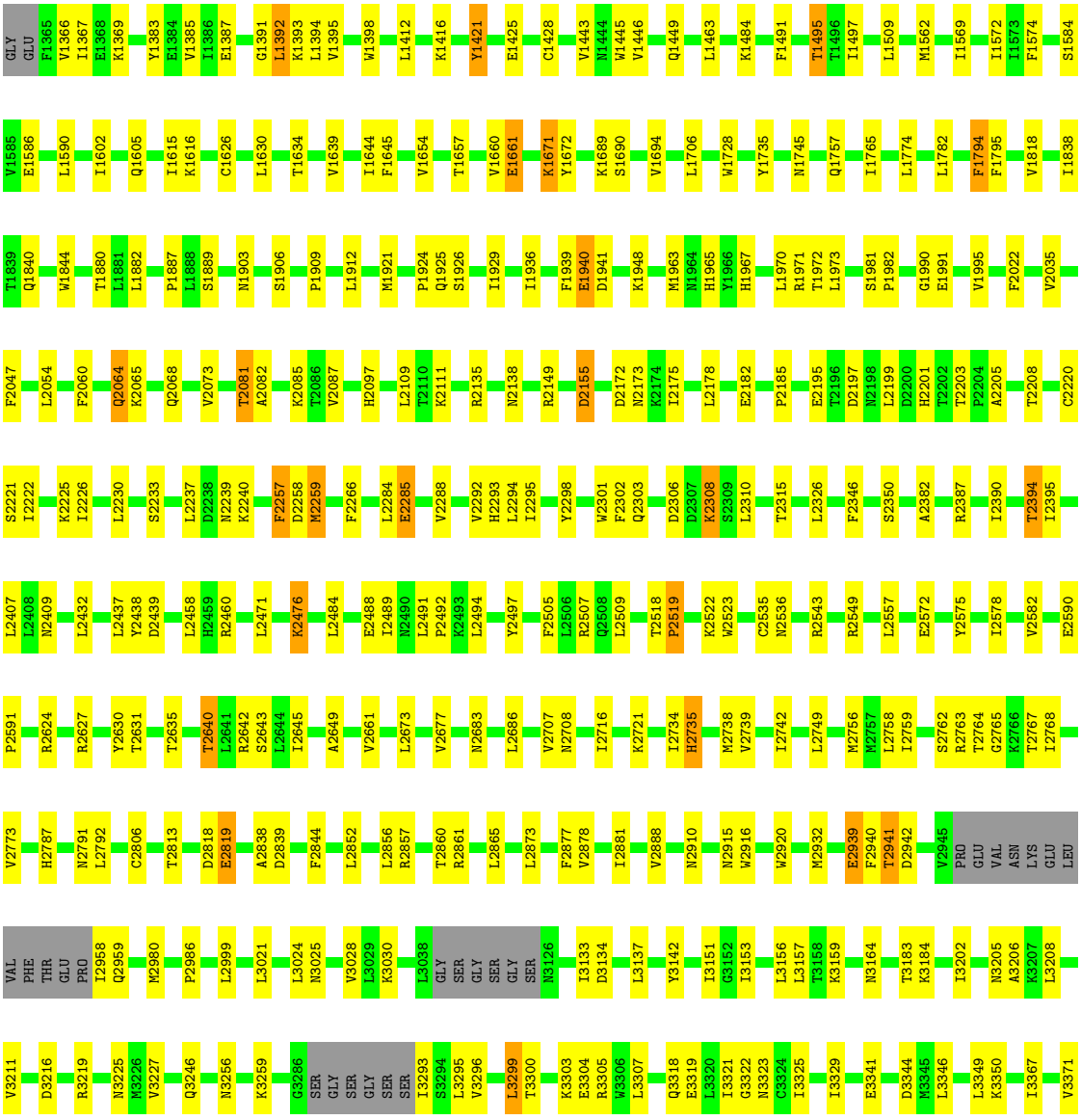
Chain	Residue	Modelled	Actual	Comment	Reference
A	4101	HIS	-	expression tag	UNP P36022
A	4102	HIS	-	expression tag	UNP P36022
A	4103	HIS	-	expression tag	UNP P36022
A	4104	HIS	-	expression tag	UNP P36022

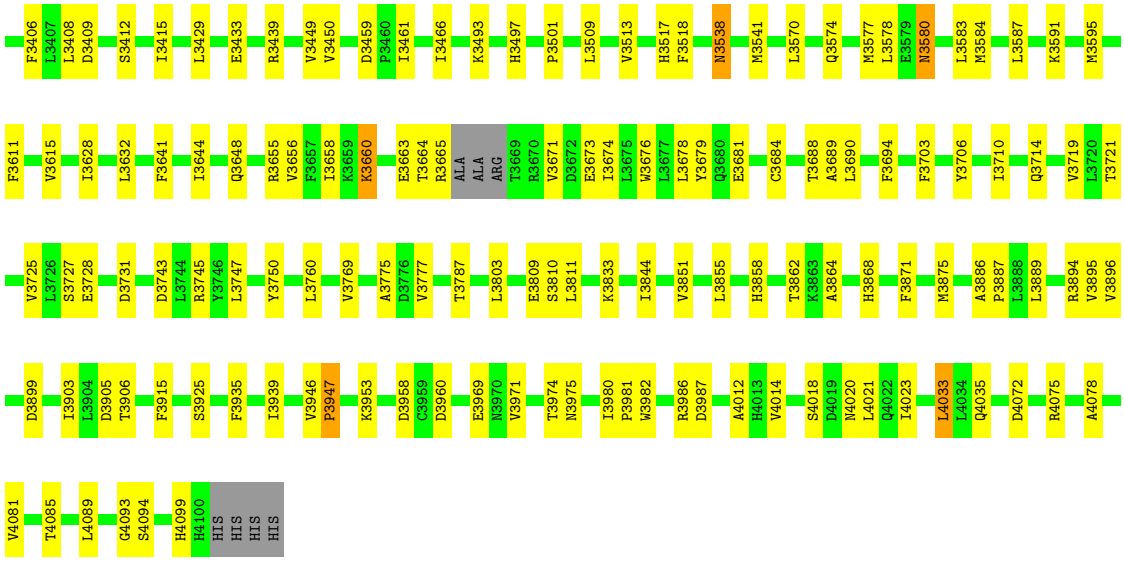
3 Residue-property plots (i)

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. 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. 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

Chain A: 81% 16% ••




F3406
L3407
L3408
D3409
S3412
I3415
L3429
E3433
R3439
V3449
V3450
D3459
P3460
I3461
I3466
K3493
H3497
P3501
L3509
V3513
H3517
F3518
N3538
M3541
L3570
Q3574
M3577
L3578
E3579
N3580
L3583
M3584
L3587
K3591
M3595
F3611
V3615
I3628
L3632
F3641
I3644
Q3648
R3655
V3656
F3657
I3658
K3659
K3660
E3663
T3664
R3665
ALA
ALA
ARG
T3669
R3670
V3671
D3672
E3673
I3674
L3675
W3676
L3677
L3678
Y3679
Q3680
E3681
C3684
T3688
A3689
L3690
F3694
F3703
Y3706
I3710
Q3714
V3719
L3720
T3721
V3725
L3726
S3727
E3728
D3731
D3743
L3744
R3745
Y3746
L3747
Y3750
L3760
V3769
A3775
D3776
V3777
T3787
L3803
E3809
S3810
L3811
K3833
I3844
V3851
L3855
H3858
T3862
K3863
A3864
H3868
F3871
M3875
A3886
P3887
L3888
L3889
R3894
V3895
V3896
D3899
I3903
L3904
D3905
T3906
F3915
S3925
F3935
I3939
V3946
P3947
K3953
D3958
C3959
D3960
E3969
N3970
V3971
T3974
N3975
I3980
P3981
W3982
R3986
D3987
A4012
H4013
V4014
S4018
D4019
N4020
L4021
Q4022
I4023
L4033
L4034
Q4035
D4072
R4075
A4078
V4081
T4085
L4089
G4093
S4094
H4099
H4100
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	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) 99.5 (47.66-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.276 , 0.320 0.276 , 0.320	Depositor DCC
R_{free} test set	1997 reflections (8.61%)	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)	0.29 , 122.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	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.*

[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	0.26	0/21632	0.44	1/29225 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2941	THR	N-CA-C	5.17	124.97	111.00

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	257	0
All	All	21212	21316	21315	257	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 (257) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2258:ASP:O	1:A:2259:MET:HB2	1.96	0.65
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3346:LEU:HD11	1:A:3350:LYS:HE3	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: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:2173:ASN:HB3	1:A:2175:ILE:HG22	1.90	0.52
1:A:1971:ARG:HB2	1:A:2208:THR:HG21	1.90	0.52
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:3760:LEU:HD21	1:A:4078:ALA:HA	1.95	0.48
1:A:1838:ILE:HD11	1:A:1844:TRP:C	2.34	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
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:2762:SER:C	1:A:2764:THR:H	2.17	0.48
1:A:3678:LEU:HD23	1:A:3678:LEU:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3658:ILE:HD12	1:A:3658:ILE:N	2.30	0.47
1:A:2980:MET:HE3	1:A:3341:GLU:HB3	1.96	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:3663:GLU:C	1:A:3665:ARG:H	2.19	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:1939:PHE:O	1:A:1940:GLU:C	2.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:3202:ILE:HG23	1:A:3208:LEU:HB2	1.99	0.44
1:A:2877:PHE:CE2	1:A:2881:ILE:HD11	2.53	0.44
1:A:3307:LEU:HD12	1:A:3307:LEU:C	2.37	0.43
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2225:LYS:NZ	1:A:2285:GLU:OE2	2.35	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
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:3256:ASN:HA	1:A:3259:LYS:HZ2	1.86	0.41
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	2.03	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:3833:LYS:HZ2	1:A:3858:HIS:CD2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2716:ILE:HD12	1:A:2739:VAL:HG22	2.02	0.40
1:A:3689:ALA:C	1:A:3690:LEU:HD12	2.42	0.40
1:A:3205:ASN:O	1:A:3206:ALA:HB3	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	2618/2661 (98%)	2464 (94%)	141 (5%)	13 (0%)	29 68

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

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Mol	Chain	Res	Type
1	A	2288	VAL

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	2381/2406 (99%)	2309 (97%)	72 (3%)	41 63

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1383	TYR
1	A	1392	LEU
1	A	1421	TYR
1	A	1463	LEU
1	A	1495	THR
1	A	1602	ILE
1	A	1605	GLN
1	A	1661	GLU
1	A	1671	LYS
1	A	1794	PHE
1	A	1818	VAL
1	A	1880	THR
1	A	1889	SER
1	A	1903	ASN
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	2172	ASP
1	A	2239	ASN
1	A	2257	PHE
1	A	2285	GLU
1	A	2295	ILE

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Mol	Chain	Res	Type
1	A	2302	PHE
1	A	2303	GLN
1	A	2308	LYS
1	A	2346	PHE
1	A	2394	THR
1	A	2439	ASP
1	A	2476	LYS
1	A	2494	LEU
1	A	2640	THR
1	A	2683	ASN
1	A	2721	LYS
1	A	2735	HIS
1	A	2767	THR
1	A	2819	GLU
1	A	2920	TRP
1	A	2932	MET
1	A	2939	GLU
1	A	2941	THR
1	A	2942	ASP
1	A	2999	LEU
1	A	3142	TYR
1	A	3164	ASN
1	A	3299	LEU
1	A	3305	ARG
1	A	3344	ASP
1	A	3538	ASN
1	A	3577	MET
1	A	3578	LEU
1	A	3580	ASN
1	A	3595	MET
1	A	3660	LYS
1	A	3714	GLN
1	A	3745	ARG
1	A	3747	LEU
1	A	3750	TYR
1	A	3871	PHE
1	A	3899	ASP
1	A	3905	ASP
1	A	3906	THR
1	A	3915	PHE
1	A	3939	ILE
1	A	3958	ASP

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Mol	Chain	Res	Type
1	A	3960	ASP
1	A	3975	ASN
1	A	3982	TRP
1	A	3987	ASP
1	A	4033	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1899	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.