Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 02:57 PM EDT

PDB ID	:	6WLG
Title	:	Ints3 C-terminal Domain
Authors	:	Li, J.; Ma, X.L.; Banerjee, S.; Dong, Z.G.
Deposited on	:	2020-04-20
Resolution	:	3.11 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:

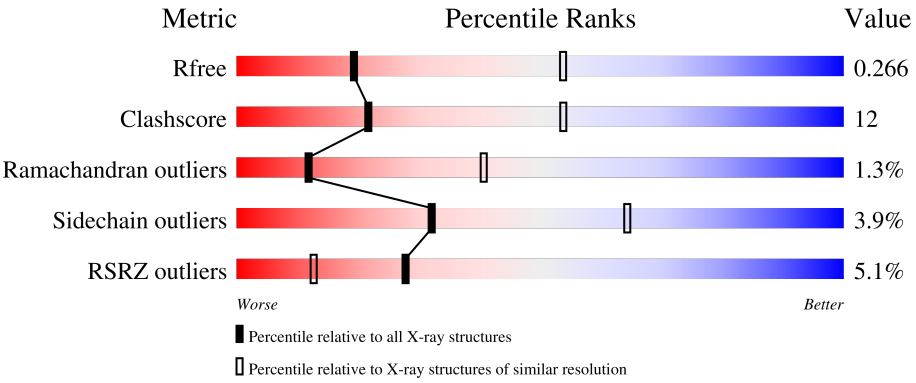
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	423	3% 60% 24% • 15%
1	B	423	6% 57% 24% • 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5750 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 Integrator complex subunit 3.

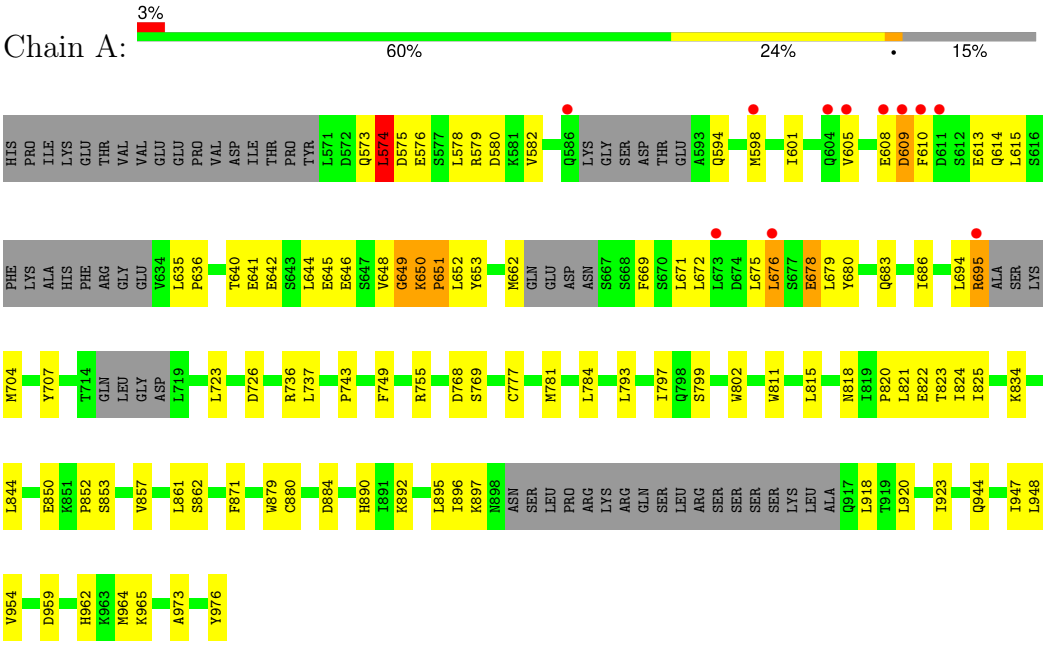
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2938	1872	481	559	26			
1	B	346	Total	C	N	O	S	0	0	0
			2812	1796	465	527	24			

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.

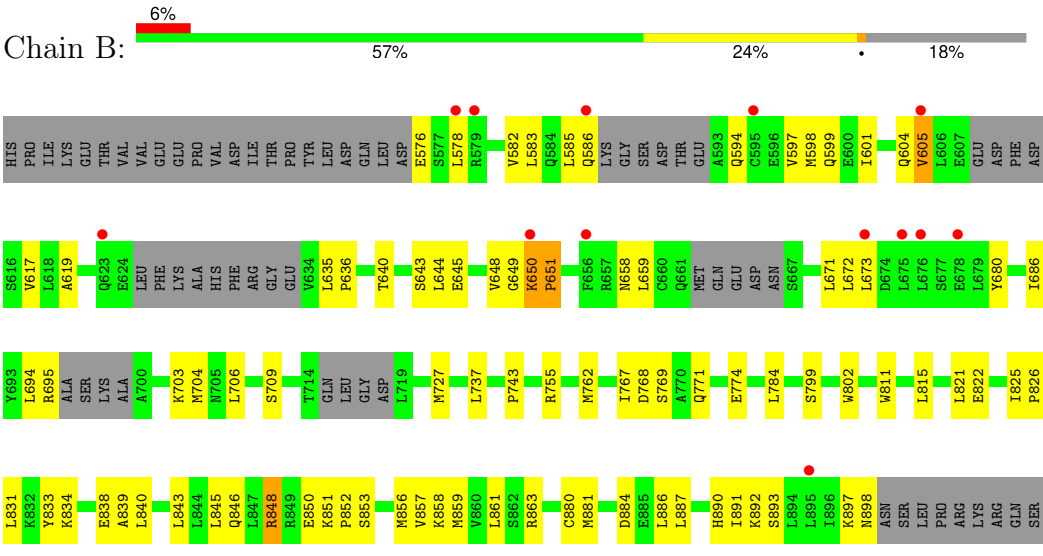
• Molecule 1: Integrator complex subunit 3

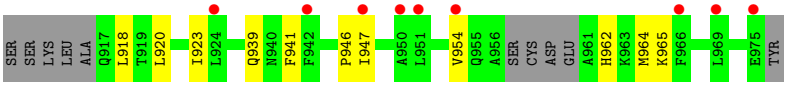
Chain A:



• Molecule 1: Integrator complex subunit 3

Chain B:




SER
SER
LYS
LEU
ALA
Q917
L918
T919
L920
I923
L924
Q939
N940
F941
F942
P946
I947
A950
L951
V954
Q955
A956
SER
CYS
ASP
GLU
A961
H962
K963
M964
K965
F966
L969
E975
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	234.85Å 234.85Å 47.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.32 – 3.11 46.32 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.32-3.11) 95.1 (46.32-3.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.204 , 0.263 0.208 , 0.266	Depositor DCC
R_{free} test set	825 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	108.0	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 119.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5750	wwPDB-VP
Average B, all atoms (Å^2)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

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	0.26	0/2986	0.48	1/4031 (0.0%)
1	B	0.26	0/2856	0.47	0/3852
All	All	0.26	0/5842	0.47	1/7883 (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	574	LEU	CA-CB-CG	5.37	127.66	115.30

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	2938	0	2931	70	0
1	B	2812	0	2830	68	0
All	All	5750	0	5761	137	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 (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:VAL:HG22	1:B:597:VAL:HG12	1.54	0.89
1:A:662:MET:HB3	1:A:669:PHE:HA	1.65	0.79
1:A:617:VAL:HG21	1:A:678:GLU:HB3	1.64	0.78
1:A:578:LEU:HD12	1:A:579:ARG:H	1.47	0.76
1:B:582:VAL:HG21	1:B:601:ILE:HD11	1.69	0.75
1:A:962:HIS:HA	1:A:965:LYS:HB3	1.67	0.75
1:B:831:LEU:HD12	1:B:840:LEU:HG	1.70	0.72
1:A:578:LEU:HD13	1:A:601:ILE:HG12	1.77	0.67
1:A:578:LEU:HD12	1:A:579:ARG:N	2.09	0.66
1:B:635:LEU:HG	1:B:737:LEU:HD23	1.76	0.66
1:B:829:GLN:HG3	1:B:859:MET:HE1	1.78	0.64
1:A:680:TYR:HB2	1:A:686:ILE:HD11	1.79	0.63
1:B:578:LEU:H	1:B:578:LEU:HD23	1.63	0.63
1:B:828:LEU:HD22	1:B:863:ARG:HD2	1.80	0.63
1:B:727:MET:HB3	1:B:762:MET:HE1	1.80	0.62
1:B:831:LEU:HD11	1:B:839:ALA:HB3	1.81	0.62
1:B:825:ILE:HG13	1:B:826:PRO:HD3	1.80	0.62
1:A:640:THR:C	1:A:642:GLU:H	2.04	0.61
1:A:694:LEU:HD13	1:A:704:MET:HG3	1.82	0.61
1:B:636:PRO:HG2	1:B:644:LEU:HA	1.81	0.61
1:B:659:LEU:HG	1:B:706:LEU:HD21	1.84	0.60
1:B:694:LEU:HD22	1:B:704:MET:HA	1.82	0.59
1:A:768:ASP:OD1	1:A:769:SER:N	2.35	0.59
1:B:893:SER:O	1:B:898:ASN:ND2	2.36	0.59
1:B:650:LYS:HB3	1:B:651:PRO:HD3	1.85	0.59
1:A:820:PRO:O	1:A:823:THR:OG1	2.21	0.58
1:A:959:ASP:HB3	1:A:962:HIS:CD2	2.39	0.57
1:A:640:THR:O	1:A:642:GLU:N	2.34	0.56
1:A:884:ASP:OD2	1:A:944:GLN:NE2	2.39	0.56
1:B:768:ASP:OD1	1:B:769:SER:N	2.37	0.56
1:B:585:LEU:HD22	1:B:594:GLN:HG3	1.88	0.55
1:A:707:TYR:OH	1:A:726:ASP:OD1	2.23	0.55
1:B:680:TYR:HB2	1:B:686:ILE:HD11	1.89	0.54
1:A:635:LEU:HG	1:A:737:LEU:HD23	1.89	0.54
1:A:799:SER:HA	1:A:802:TRP:CE2	2.42	0.54
1:B:887:LEU:O	1:B:891:ILE:HG12	2.08	0.54
1:A:844:LEU:HG	1:A:871:PHE:CD2	2.43	0.53
1:B:583:LEU:HD21	1:B:619:ALA:HB1	1.90	0.53
1:A:645:GLU:HA	1:A:648:VAL:HG12	1.90	0.53
1:B:799:SER:HA	1:B:802:TRP:CE2	2.42	0.53
1:A:861:LEU:HD13	1:A:923:ILE:HG23	1.90	0.53
1:A:576:GLU:H	1:A:579:ARG:NH2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:TRP:O	1:A:815:LEU:HG	2.10	0.52
1:B:640:THR:OG1	1:B:643:SER:HB2	2.09	0.52
1:B:852:PRO:HA	1:B:856:MET:HE2	1.91	0.52
1:A:880:CYS:O	1:A:884:ASP:HB3	2.10	0.52
1:B:920:LEU:HD11	1:B:954:VAL:HG13	1.92	0.52
1:B:767:ILE:HG13	1:B:771:GLN:HB2	1.92	0.51
1:A:884:ASP:OD1	1:A:884:ASP:N	2.40	0.51
1:A:920:LEU:HD11	1:A:954:VAL:HG13	1.91	0.51
1:B:821:LEU:HD11	1:B:846:GLN:HB3	1.92	0.51
1:B:586:GLN:HE21	1:B:594:GLN:HG2	1.76	0.50
1:A:617:VAL:HG12	1:A:675:LEU:HD12	1.94	0.50
1:B:755:ARG:HA	1:B:755:ARG:NE	2.26	0.50
1:A:617:VAL:HB	1:A:679:LEU:HD22	1.94	0.49
1:A:613:GLU:O	1:A:617:VAL:HG13	2.12	0.49
1:B:743:PRO:HA	1:B:784:LEU:HD13	1.94	0.49
1:B:601:ILE:O	1:B:605:VAL:HG23	2.12	0.49
1:B:880:CYS:HB2	1:B:941:PHE:CD1	2.47	0.49
1:A:636:PRO:HG2	1:A:644:LEU:HA	1.94	0.49
1:A:880:CYS:HA	1:A:884:ASP:HA	1.96	0.48
1:B:650:LYS:HB3	1:B:651:PRO:CD	2.43	0.48
1:A:576:GLU:H	1:A:579:ARG:HH21	1.60	0.48
1:B:582:VAL:HG21	1:B:601:ILE:CD1	2.42	0.48
1:A:892:LYS:HG3	1:A:950:ALA:HB2	1.97	0.47
1:B:821:LEU:O	1:B:825:ILE:HG23	2.14	0.47
1:A:646:GLU:O	1:A:650:LYS:NZ	2.35	0.47
1:A:793:LEU:HD13	1:A:824:ILE:HA	1.95	0.47
1:B:771:GLN:HA	1:B:774:GLU:HG2	1.96	0.47
1:A:838:GLU:H	1:A:838:GLU:CD	2.18	0.47
1:A:582:VAL:HG21	1:A:601:ILE:HD11	1.98	0.46
1:B:811:TRP:O	1:B:815:LEU:HG	2.14	0.46
1:A:614:GLN:HG2	1:A:615:LEU:HD12	1.97	0.46
1:A:723:LEU:HD11	1:A:749:PHE:CD2	2.50	0.46
1:A:793:LEU:O	1:A:797:ILE:HG13	2.15	0.46
1:B:962:HIS:O	1:B:965:LYS:HB3	2.16	0.46
1:A:594:GLN:N	1:A:594:GLN:OE1	2.49	0.46
1:B:690:LEU:HD11	1:B:706:LEU:HD12	1.98	0.46
1:B:822:GLU:HA	1:B:825:ILE:HG12	1.98	0.46
1:B:829:GLN:HG3	1:B:859:MET:CE	2.46	0.45
1:B:645:GLU:O	1:B:648:VAL:HG12	2.16	0.45
1:B:703:LYS:HD3	1:B:703:LYS:HA	1.67	0.45
1:B:578:LEU:O	1:B:582:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:GLN:O	1:A:947:ILE:HG22	2.17	0.45
1:A:635:LEU:HD12	1:A:736:ARG:HG2	1.99	0.45
1:B:884:ASP:N	1:B:884:ASP:OD1	2.48	0.45
1:B:880:CYS:HB3	1:B:887:LEU:HD23	1.98	0.45
1:B:947:ILE:HD12	1:B:947:ILE:HA	1.82	0.45
1:A:948:LEU:HD22	1:A:973:ALA:HA	1.99	0.45
1:B:582:VAL:HG22	1:B:597:VAL:CG1	2.37	0.45
1:A:918:LEU:HD13	1:A:923:ILE:HD11	1.98	0.44
1:B:853:SER:OG	1:B:856:MET:HG3	2.17	0.44
1:B:838:GLU:H	1:B:838:GLU:CD	2.21	0.44
1:A:601:ILE:O	1:A:605:VAL:HG23	2.18	0.44
1:B:598:MET:HA	1:B:601:ILE:HD12	1.99	0.44
1:B:881:MET:HG2	1:B:939:GLN:HG3	1.98	0.44
1:B:821:LEU:HD12	1:B:850:GLU:HG3	2.00	0.44
1:B:845:LEU:HA	1:B:848:ARG:HD2	2.00	0.43
1:B:614:GLN:HA	1:B:617:VAL:HG22	1.99	0.43
1:A:676:LEU:HD23	1:A:676:LEU:H	1.84	0.43
1:A:755:ARG:HD2	1:B:829:GLN:HB3	2.00	0.43
1:B:918:LEU:HD23	1:B:918:LEU:HA	1.75	0.43
1:A:777:CYS:O	1:A:781:MET:HG3	2.18	0.43
1:A:839:ALA:O	1:A:843:LEU:HB2	2.19	0.43
1:A:895:LEU:HD22	1:A:954:VAL:HG21	2.01	0.43
1:B:851:LYS:HE3	1:B:886:LEU:HD22	2.01	0.43
1:A:649:GLY:O	1:A:653:TYR:HB2	2.18	0.43
1:A:676:LEU:HA	1:A:679:LEU:HB2	2.01	0.43
1:A:640:THR:C	1:A:642:GLU:N	2.70	0.43
1:A:821:LEU:HD12	1:A:850:GLU:HG3	1.99	0.42
1:B:858:LYS:HG3	1:B:918:LEU:HD12	2.00	0.42
1:A:679:LEU:O	1:A:683:GLN:N	2.49	0.42
1:B:599:GLN:HE22	1:B:658:ASN:HD21	1.68	0.42
1:A:844:LEU:HG	1:A:871:PHE:CE2	2.54	0.42
1:A:609:ASP:OD2	1:A:609:ASP:N	2.53	0.42
1:A:896:ILE:HG23	1:A:953:HIS:CE1	2.54	0.42
1:A:834:LYS:HD3	1:A:834:LYS:HA	1.73	0.42
1:B:857:VAL:HG21	1:B:890:HIS:HB3	2.02	0.42
1:B:635:LEU:HD23	1:B:635:LEU:HA	1.93	0.41
1:B:706:LEU:O	1:B:709:SER:OG	2.27	0.41
1:A:695:ARG:C	1:A:695:ARG:HH11	2.24	0.41
1:A:574:LEU:HD21	1:A:580:ASP:OD2	2.21	0.41
1:A:743:PRO:HA	1:A:784:LEU:HD13	2.02	0.41
1:A:852:PRO:HB3	1:A:879:TRP:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:SER:OG	1:A:918:LEU:HG	2.21	0.41
1:A:918:LEU:HA	1:A:918:LEU:HD23	1.84	0.41
1:B:833:TYR:CD2	1:B:834:LYS:HG2	2.56	0.41
1:B:861:LEU:HD13	1:B:923:ILE:HG23	2.03	0.41
1:A:703:LYS:HD3	1:A:703:LYS:HA	1.82	0.41
1:A:650:LYS:HB3	1:A:651:PRO:CD	2.51	0.40
1:B:576:GLU:HG3	1:B:578:LEU:CD2	2.50	0.40
1:B:582:VAL:HA	1:B:597:VAL:CG1	2.51	0.40
1:A:822:GLU:O	1:A:825:ILE:HG22	2.21	0.40
1:A:959:ASP:HB3	1:A:962:HIS:HD2	1.85	0.40
1:B:692:TYR:CD1	1:B:737:LEU:HD21	2.56	0.40
1:A:857:VAL:HG21	1:A:890:HIS:HB3	2.03	0.40
1:B:892:LYS:HD2	1:B:946:PRO:HB3	2.02	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	347/423 (82%)	317 (91%)	25 (7%)	5 (1%)	11	39
1	B	328/423 (78%)	305 (93%)	19 (6%)	4 (1%)	13	43
All	All	675/846 (80%)	622 (92%)	44 (6%)	9 (1%)	12	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	641	GLU
1	A	649	GLY
1	B	649	GLY
1	B	650	LYS
1	B	651	PRO

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Mol	Chain	Res	Type
1	A	575	ASP
1	A	651	PRO
1	A	650	LYS
1	B	605	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	339/394 (86%)	322 (95%)	17 (5%)	24	56
1	B	324/394 (82%)	315 (97%)	9 (3%)	43	72
All	All	663/788 (84%)	637 (96%)	26 (4%)	32	64

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	GLN
1	A	574	LEU
1	A	598	MET
1	A	608	GLU
1	A	609	ASP
1	A	610	PHE
1	A	652	LEU
1	A	671	LEU
1	A	672	LEU
1	A	676	LEU
1	A	678	GLU
1	A	695	ARG
1	A	818	ASN
1	A	853	SER
1	A	897	LYS
1	A	964	MET
1	A	976	TYR
1	B	604	GLN
1	B	671	LEU

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Mol	Chain	Res	Type
1	B	672	LEU
1	B	673	LEU
1	B	695	ARG
1	B	843	LEU
1	B	848	ARG
1	B	897	LYS
1	B	964	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	818	ASN
1	A	866	HIS
1	A	962	HIS
1	B	623	GLN
1	B	658	ASN
1	B	761	ASN
1	B	798	GLN
1	B	829	GLN
1	B	883	HIS
1	B	917	GLN
1	B	936	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

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, 95^{th} 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	361/423 (85%)	0.01	11 (3%) 50 27	67, 124, 240, 371	0
1	B	346/423 (81%)	0.30	25 (7%) 15 6	79, 153, 273, 347	0
All	All	707/846 (83%)	0.15	36 (5%) 28 13	67, 138, 266, 371	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	595	CYS	8.7
1	B	975	GLU	6.0
1	B	676	LEU	5.9
1	B	673	LEU	4.8
1	B	678	GLU	4.4
1	B	969	LEU	4.3
1	B	614	GLN	4.2
1	A	611	ASP	4.0
1	A	586	GLN	3.5
1	A	676	LEU	3.4
1	B	954	VAL	3.4
1	A	604	GLN	3.3
1	B	951	LEU	3.3
1	A	610	PHE	3.3
1	B	623	GLN	3.2
1	B	942	PHE	3.2
1	B	612	SER	3.1
1	A	605	VAL	3.0
1	B	615	LEU	3.0
1	B	578	LEU	3.0
1	B	966	PHE	3.0
1	A	608	GLU	2.9
1	B	605	VAL	2.9
1	B	579	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	895	LEU	2.8
1	B	656	PHE	2.7
1	B	947	ILE	2.7
1	A	609	ASP	2.7
1	A	673	LEU	2.5
1	A	695	ARG	2.4
1	B	675	LEU	2.3
1	B	950	ALA	2.3
1	B	586	GLN	2.1
1	A	598	MET	2.1
1	B	650	LYS	2.1
1	B	924	LEU	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.