Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 01:39 PM EST

PDB ID	:	4M8M
Title	:	Crystal structure of the active dimer of zebrafish PlexinC1 cytoplasmic region
Authors	:	Wang, Y.; Pascoe, H.G.; Zhang, X.
Deposited on	:	2013-08-13
Resolution	:	3.31 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:

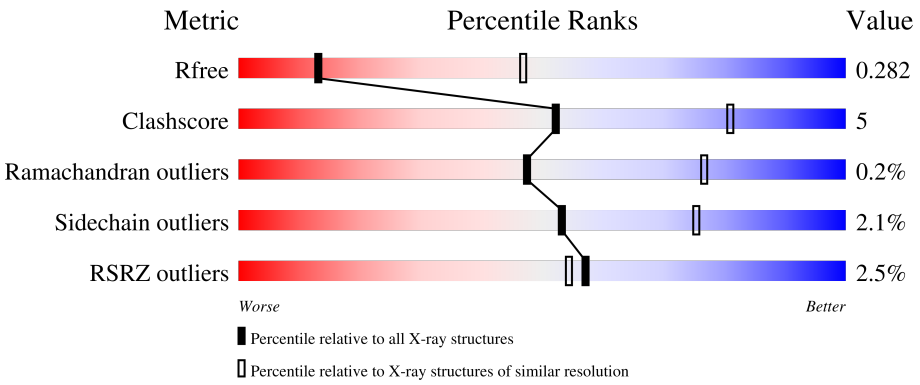
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.31 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	632	2% 79% 12% 9%
1	B	632	2% 76% 14% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8888 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 GCN4 coiled-coil fused zebrafish PlexinC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	573	4449	2867	737	824	21	0	0	0
1	B	574	4422	2854	732	815	21	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	522	GLY	-	expression tag	UNP Q5RGW1
A	523	GLY	-	expression tag	UNP Q5RGW1
A	524	SER	-	expression tag	UNP Q5RGW1
A	525	VAL	-	expression tag	UNP Q5RGW1
A	526	LYS	-	expression tag	UNP Q5RGW1
A	527	GLN	-	expression tag	UNP Q5RGW1
A	528	LEU	-	expression tag	UNP Q5RGW1
A	529	GLU	-	expression tag	UNP Q5RGW1
A	530	ASP	-	expression tag	UNP Q5RGW1
A	531	LYS	-	expression tag	UNP Q5RGW1
A	532	VAL	-	expression tag	UNP Q5RGW1
A	533	GLU	-	expression tag	UNP Q5RGW1
A	534	GLU	-	expression tag	UNP Q5RGW1
A	535	LEU	-	expression tag	UNP Q5RGW1
A	536	LEU	-	expression tag	UNP Q5RGW1
A	537	SER	-	expression tag	UNP Q5RGW1
A	538	LYS	-	expression tag	UNP Q5RGW1
A	539	ASN	-	expression tag	UNP Q5RGW1
A	540	ALA	-	expression tag	UNP Q5RGW1
A	541	HIS	-	expression tag	UNP Q5RGW1
A	542	LEU	-	expression tag	UNP Q5RGW1
A	543	GLU	-	expression tag	UNP Q5RGW1
A	544	ASN	-	expression tag	UNP Q5RGW1
A	545	GLU	-	expression tag	UNP Q5RGW1
A	546	VAL	-	expression tag	UNP Q5RGW1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	547	ALA	-	expression tag	UNP Q5RGW1
A	548	ARG	-	expression tag	UNP Q5RGW1
A	549	LEU	-	expression tag	UNP Q5RGW1
A	550	LYS	-	expression tag	UNP Q5RGW1
A	551	LYS	-	expression tag	UNP Q5RGW1
A	552	LEU	-	expression tag	UNP Q5RGW1
B	522	GLY	-	expression tag	UNP Q5RGW1
B	523	GLY	-	expression tag	UNP Q5RGW1
B	524	SER	-	expression tag	UNP Q5RGW1
B	525	VAL	-	expression tag	UNP Q5RGW1
B	526	LYS	-	expression tag	UNP Q5RGW1
B	527	GLN	-	expression tag	UNP Q5RGW1
B	528	LEU	-	expression tag	UNP Q5RGW1
B	529	GLU	-	expression tag	UNP Q5RGW1
B	530	ASP	-	expression tag	UNP Q5RGW1
B	531	LYS	-	expression tag	UNP Q5RGW1
B	532	VAL	-	expression tag	UNP Q5RGW1
B	533	GLU	-	expression tag	UNP Q5RGW1
B	534	GLU	-	expression tag	UNP Q5RGW1
B	535	LEU	-	expression tag	UNP Q5RGW1
B	536	LEU	-	expression tag	UNP Q5RGW1
B	537	SER	-	expression tag	UNP Q5RGW1
B	538	LYS	-	expression tag	UNP Q5RGW1
B	539	ASN	-	expression tag	UNP Q5RGW1
B	540	ALA	-	expression tag	UNP Q5RGW1
B	541	HIS	-	expression tag	UNP Q5RGW1
B	542	LEU	-	expression tag	UNP Q5RGW1
B	543	GLU	-	expression tag	UNP Q5RGW1
B	544	ASN	-	expression tag	UNP Q5RGW1
B	545	GLU	-	expression tag	UNP Q5RGW1
B	546	VAL	-	expression tag	UNP Q5RGW1
B	547	ALA	-	expression tag	UNP Q5RGW1
B	548	ARG	-	expression tag	UNP Q5RGW1
B	549	LEU	-	expression tag	UNP Q5RGW1
B	550	LYS	-	expression tag	UNP Q5RGW1
B	551	LYS	-	expression tag	UNP Q5RGW1
B	552	LEU	-	expression tag	UNP Q5RGW1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	11	11	11	0	0

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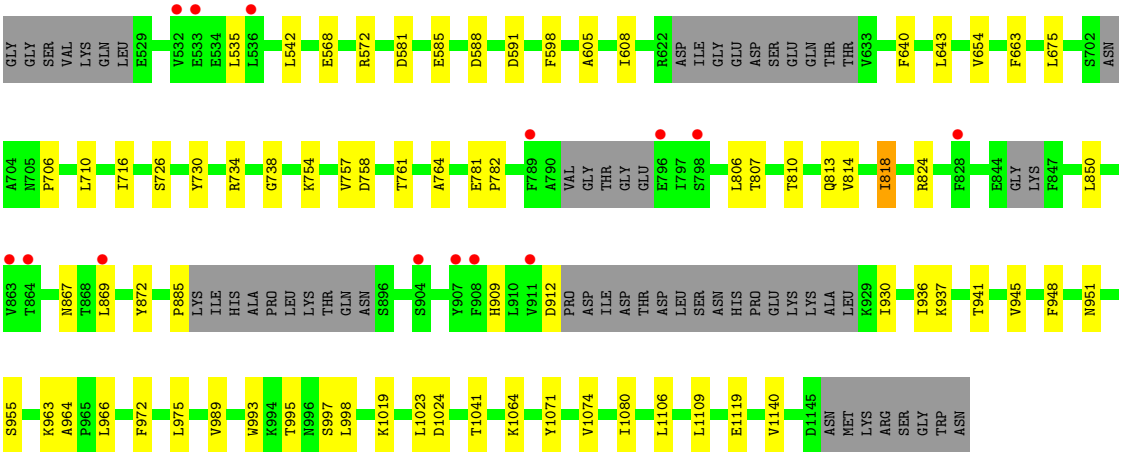
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	6	6	6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

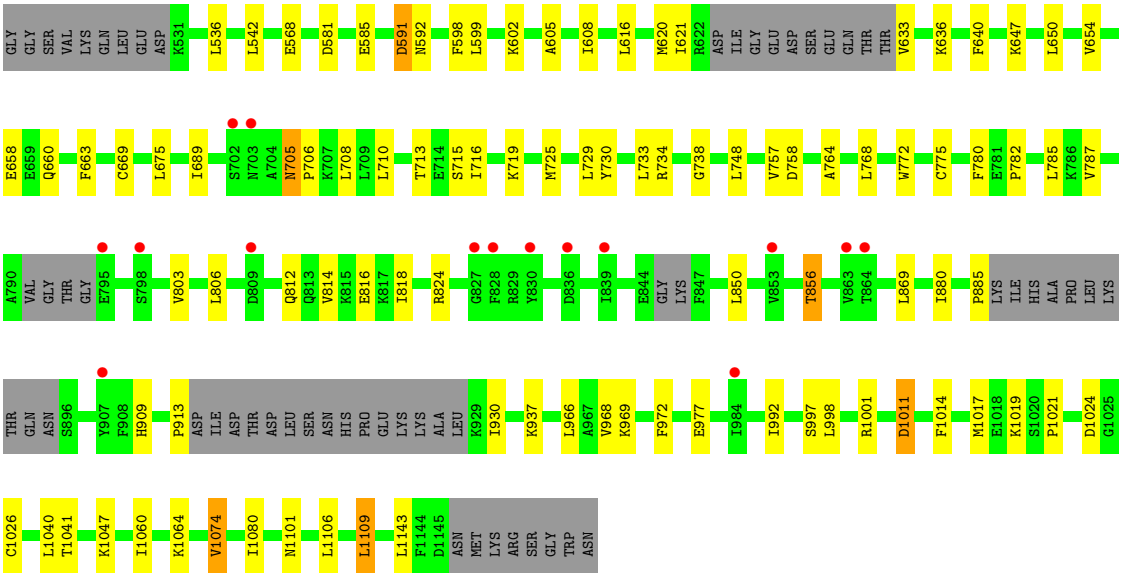
• Molecule 1: GCN4 coiled-coil fused zebrafish PlexinC1

Chain A: 2% 79% 12% 9%



• Molecule 1: GCN4 coiled-coil fused zebrafish PlexinC1

Chain B: 2% 76% 14% • 9%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.22Å 146.10Å 209.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.16 – 3.31 44.16 – 3.31	Depositor EDS
% Data completeness (in resolution range)	83.3 (44.16-3.31) 83.5 (44.16-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.226 , 0.281 0.225 , 0.282	Depositor DCC
R_{free} test set	1074 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	77.8	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8888	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8818e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.32	0/4530	0.47	1/6130 (0.0%)
1	B	0.30	0/4504	0.47	2/6103 (0.0%)
All	All	0.31	0/9034	0.47	3/12233 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	913	PRO	N-CA-CB	5.94	110.43	103.30
1	B	885	PRO	N-CA-CB	5.74	110.19	103.30
1	A	885	PRO	N-CA-CB	5.71	110.16	103.30

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	4449	0	4280	42	0
1	B	4422	0	4224	56	0
2	A	11	0	0	0	0
2	B	6	0	0	0	0
All	All	8888	0	8504	95	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 5.

All (95) 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:966:LEU:HG	1:B:1080:ILE:HD13	1.68	0.76
1:B:713:THR:OG1	1:B:1001:ARG:NH2	2.21	0.74
1:A:654:VAL:HG13	1:A:716:ILE:HD12	1.68	0.73
1:A:972:PHE:HD2	1:A:1074:VAL:HG11	1.59	0.68
1:B:654:VAL:HG13	1:B:716:ILE:HD12	1.76	0.67
1:A:588:ASP:OD2	1:A:754:LYS:NZ	2.27	0.67
1:A:535:LEU:HD11	1:B:536:LEU:HD23	1.81	0.63
1:B:787:VAL:HG22	1:B:880:ILE:HB	1.82	0.62
1:B:1041:THR:O	1:B:1064:LYS:NZ	2.32	0.62
1:A:568:GLU:OE2	1:A:572:ARG:NH2	2.34	0.60
1:B:605:ALA:HA	1:B:608:ILE:HG22	1.84	0.59
1:A:605:ALA:HA	1:A:608:ILE:HG22	1.83	0.58
1:A:814:VAL:HG21	1:A:869:LEU:HD21	1.86	0.56
1:B:1019:LYS:HE2	1:B:1024:ASP:HB2	1.88	0.56
1:B:768:LEU:HD12	1:B:1026:CYS:HB3	1.87	0.56
1:A:930:ILE:HD11	1:B:568:GLU:HG3	1.88	0.55
1:B:782:PRO:HA	1:B:806:LEU:HD23	1.89	0.55
1:A:1019:LYS:HE2	1:A:1024:ASP:HB2	1.89	0.55
1:A:758:ASP:OD2	1:A:761:THR:OG1	2.23	0.54
1:B:757:VAL:HG22	1:B:764:ALA:HB2	1.89	0.54
1:A:966:LEU:HG	1:A:1080:ILE:HD13	1.89	0.54
1:B:814:VAL:O	1:B:818:ILE:HG22	2.07	0.54
1:A:675:LEU:HD23	1:A:1109:LEU:HD11	1.88	0.54
1:A:640:PHE:HD2	1:A:1106:LEU:HD22	1.73	0.53
1:A:814:VAL:O	1:A:818:ILE:HG22	2.09	0.53
1:B:780:PHE:HD2	1:B:806:LEU:HD22	1.74	0.52
1:A:757:VAL:HG13	1:A:764:ALA:HB2	1.92	0.52
1:A:568:GLU:HG3	1:B:930:ILE:HD11	1.92	0.52
1:B:650:LEU:HD23	1:B:689:ILE:HG12	1.92	0.51
1:A:643:LEU:HD22	1:A:1140:VAL:HG21	1.92	0.51
1:B:730:TYR:CE2	1:B:734:ARG:HD2	2.45	0.51
1:A:598:PHE:HZ	1:A:738:GLY:HA3	1.76	0.50
1:A:706:PRO:O	1:A:993:TRP:NE1	2.43	0.50
1:A:591:ASP:HB3	1:A:824:ARG:HB3	1.94	0.50
1:B:1019:LYS:NZ	1:B:1024:ASP:OD1	2.40	0.50
1:A:1041:THR:O	1:A:1064:LYS:NZ	2.44	0.50
1:B:633:VAL:HA	1:B:636:LYS:HE2	1.93	0.49
1:B:856:THR:OG1	1:B:856:THR:O	2.25	0.49
1:A:591:ASP:OD2	1:A:824:ARG:HD2	2.13	0.49
1:A:867:ASN:HB3	1:A:872:TYR:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:HD13	1:A:997:SER:HB3	1.95	0.49
1:A:640:PHE:HD1	1:A:1140:VAL:HG11	1.78	0.48
1:B:640:PHE:HD2	1:B:1106:LEU:HD22	1.78	0.48
1:B:758:ASP:OD1	1:B:909:HIS:HB3	2.14	0.48
1:A:581:ASP:O	1:A:585:GLU:HG2	2.14	0.47
1:A:941:THR:O	1:A:945:VAL:HG23	2.14	0.47
1:B:658:GLU:OE1	1:B:715:SER:HB2	2.14	0.47
1:B:803:VAL:HG21	1:B:818:ILE:HD13	1.97	0.47
1:B:1060:ILE:HD13	1:B:1060:ILE:HA	1.78	0.46
1:B:598:PHE:HZ	1:B:738:GLY:HA3	1.81	0.46
1:B:729:LEU:HD21	1:B:968:VAL:HG23	1.97	0.46
1:A:608:ILE:HD13	1:A:726:SER:HB3	1.98	0.45
1:B:710:LEU:HD13	1:B:997:SER:HB3	1.99	0.45
1:B:660:GLN:HB2	1:B:663:PHE:HB2	1.98	0.44
1:B:785:LEU:HD13	1:B:880:ILE:HD12	1.99	0.44
1:B:937:LYS:HD3	1:B:937:LYS:HA	1.82	0.44
1:B:669:CYS:HA	1:B:719:LYS:HG2	1.99	0.44
1:A:975:LEU:HA	1:A:975:LEU:HD23	1.73	0.44
1:B:869:LEU:HD23	1:B:869:LEU:HA	1.80	0.44
1:B:748:LEU:HD23	1:B:748:LEU:HA	1.83	0.43
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.82	0.43
1:B:705:ASN:O	1:B:708:LEU:HG	2.17	0.43
1:A:963:LYS:HG2	1:A:964:ALA:O	2.18	0.43
1:B:591:ASP:OD2	1:B:824:ARG:HD2	2.19	0.43
1:B:730:TYR:O	1:B:733:LEU:HB3	2.19	0.43
1:B:972:PHE:HD2	1:B:1074:VAL:HG11	1.83	0.43
1:A:810:THR:HB	1:A:813:GLN:HG3	2.00	0.43
1:A:782:PRO:HA	1:A:806:LEU:HD23	2.01	0.42
1:B:1047:LYS:HE2	1:B:1047:LYS:HB3	1.81	0.42
1:A:542:LEU:HD23	1:A:542:LEU:HA	1.77	0.42
1:B:1014:PHE:HB2	1:B:1017:MET:HE3	2.01	0.42
1:B:602:LYS:HD2	1:B:621:ILE:HG23	2.00	0.42
1:B:812:GLN:O	1:B:816:GLU:HG3	2.20	0.42
1:B:1040:LEU:HD12	1:B:1040:LEU:HA	1.83	0.42
1:B:689:ILE:HD12	1:B:689:ILE:HA	1.87	0.42
1:B:647:LYS:HG2	1:B:689:ILE:HD13	2.02	0.41
1:A:598:PHE:CZ	1:A:734:ARG:HA	2.56	0.41
1:A:948:PHE:O	1:A:951:ASN:HB2	2.20	0.41
1:A:937:LYS:HD3	1:A:937:LYS:HA	1.75	0.41
1:A:758:ASP:OD1	1:A:909:HIS:HB3	2.21	0.41
1:A:706:PRO:HB2	1:A:989:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.94	0.41
1:A:1119:GLU:OE1	1:A:1119:GLU:N	2.40	0.41
1:B:772:TRP:HH2	1:B:1021:PRO:HB2	1.85	0.41
1:B:992:ILE:HA	1:B:992:ILE:HD13	1.82	0.41
1:B:1011:ASP:HA	1:B:1017:MET:HG2	2.03	0.41
1:A:730:TYR:CE2	1:A:734:ARG:HD2	2.57	0.41
1:B:705:ASN:HA	1:B:706:PRO:HD3	1.87	0.41
1:B:725:MET:O	1:B:729:LEU:HB2	2.21	0.41
1:B:969:LYS:HB3	1:B:1080:ILE:HD11	2.03	0.41
1:B:581:ASP:O	1:B:585:GLU:HG2	2.21	0.40
1:A:995:THR:HG22	1:A:1071:TYR:OH	2.21	0.40
1:B:675:LEU:HD23	1:B:1109:LEU:HD11	2.03	0.40
1:A:781:GLU:O	1:A:807:THR:HG23	2.22	0.40
1:B:620:MET:HA	1:B:1101:ASN:HD21	1.86	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	559/632 (88%)	516 (92%)	42 (8%)	1 (0%)	47 77
1	B	562/632 (89%)	510 (91%)	51 (9%)	1 (0%)	47 77
All	All	1121/1264 (89%)	1026 (92%)	93 (8%)	2 (0%)	47 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	998	LEU
1	A	998	LEU

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	462/582 (79%)	455 (98%)	7 (2%)	65	81
1	B	452/582 (78%)	440 (97%)	12 (3%)	44	71
All	All	914/1164 (78%)	895 (98%)	19 (2%)	53	75

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	663	PHE
1	A	818	ILE
1	A	850	LEU
1	A	912	ASP
1	A	936	ILE
1	A	955	SER
1	A	1023	LEU
1	B	591	ASP
1	B	592	ASN
1	B	616	LEU
1	B	705	ASN
1	B	775	CYS
1	B	850	LEU
1	B	856	THR
1	B	977	GLU
1	B	1011	ASP
1	B	1074	VAL
1	B	1109	LEU
1	B	1143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	723	ASN
1	A	750	GLN
1	B	603	HIS

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Mol	Chain	Res	Type
1	B	680	HIS
1	B	813	GLN
1	B	867	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	573/632 (90%)	-0.01	14 (2%)	59	56	39, 100, 164, 196	0
1	B	574/632 (90%)	0.02	15 (2%)	56	53	42, 97, 160, 209	0
All	All	1147/1264 (90%)	0.00	29 (2%)	57	54	39, 98, 162, 209	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	795	GLU	6.5
1	A	864	THR	5.4
1	A	796	GLU	4.4
1	A	798	SER	3.8
1	A	532	VAL	3.8
1	B	828	PHE	3.5
1	A	907	TYR	3.4
1	B	907	TYR	3.1
1	A	904	SER	3.1
1	B	864	THR	3.1
1	A	863	VAL	3.0
1	B	839	ILE	2.8
1	A	908	PHE	2.8
1	B	853	VAL	2.7
1	B	809	ASP	2.7
1	A	533	GLU	2.5
1	B	702	SER	2.5
1	B	798	SER	2.5
1	A	536	LEU	2.4
1	B	830	TYR	2.3
1	B	863	VAL	2.3
1	A	828	PHE	2.3
1	B	827	GLY	2.2
1	A	869	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	703	ASN	2.1
1	B	984	ILE	2.1
1	B	836	ASP	2.1
1	A	911	VAL	2.0
1	A	789	PHE	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.