Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:06 am BST

PDB ID	:	3WXF
Title	:	Crystal structure of CYLD USP domain (C596S E674Q) in complex with Met1-linked diubiquitin
Authors	:	Sato, Y.; Fukai, S.
Deposited on	:	2014-07-30
Resolution	:	2.30 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 following versions of software and data (see references ①) were used in the production of this report:

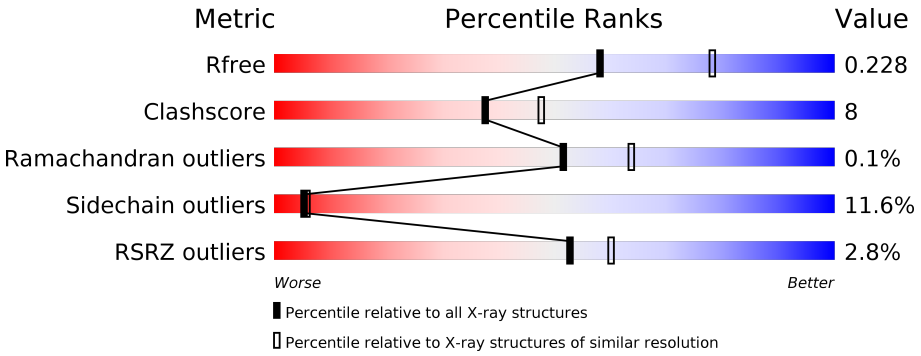
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	312	74% 17%
1	C	312	74% 17% 5%
2	B	148	4% 80% 18%
2	D	148	12% 68% 25% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7358 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2425	1560	397	447	21			
1	C	299	Total	C	N	O	S	0	0	0
			2426	1561	398	447	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP E7FEV5
A	576	HIS	-	expression tag	UNP E7FEV5
A	577	MET	-	expression tag	UNP E7FEV5
A	596	SER	CYS	engineered mutation	UNP E7FEV5
A	674	GLN	GLU	engineered mutation	UNP E7FEV5
A	781	LEU	-	linker	UNP E7FEV5
A	782	GLU	-	linker	UNP E7FEV5
A	783	GLY	-	linker	UNP E7FEV5
A	784	GLY	-	linker	UNP E7FEV5
C	575	SER	-	expression tag	UNP E7FEV5
C	576	HIS	-	expression tag	UNP E7FEV5
C	577	MET	-	expression tag	UNP E7FEV5
C	596	SER	CYS	engineered mutation	UNP E7FEV5
C	674	GLN	GLU	engineered mutation	UNP E7FEV5
C	781	LEU	-	linker	UNP E7FEV5
C	782	GLU	-	linker	UNP E7FEV5
C	783	GLY	-	linker	UNP E7FEV5
C	784	GLY	-	linker	UNP E7FEV5

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1175	740	203	230	2			

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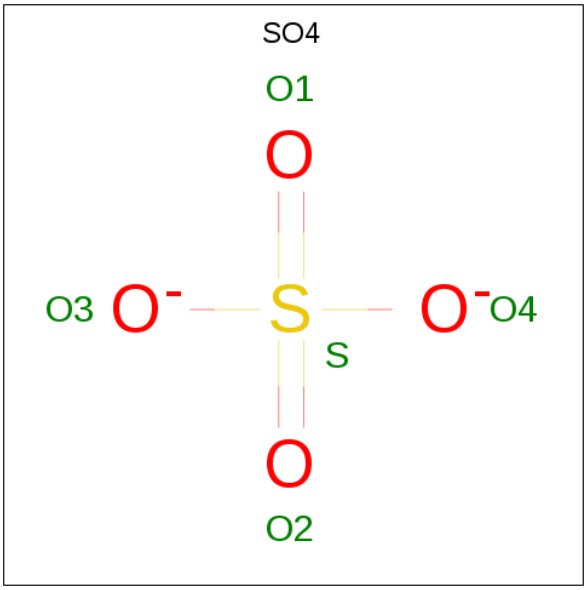
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	148	Total	C	N	O	S	0	0	0
			1175	740	203	230	2			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	O	S		0	0
			5	4	1			
3	C	1	Total	O	S		0	0
			5	4	1			

- Molecule 4 is water.

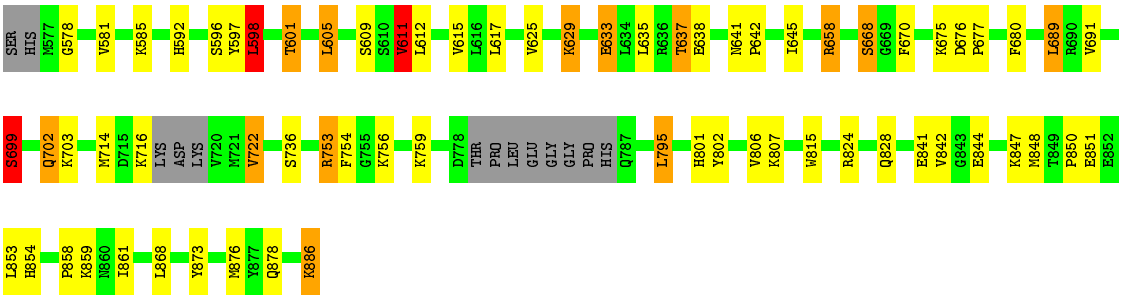
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	12	Total	O	0	0
			12	12		
4	C	60	Total	O	0	0
			60	60		
4	D	14	Total	O	0	0
			14	14		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

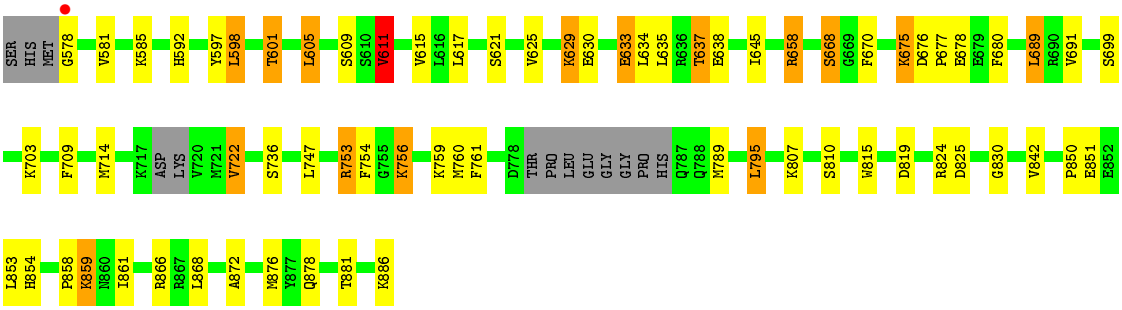
- Molecule 1: Uncharacterized protein

Chain A:



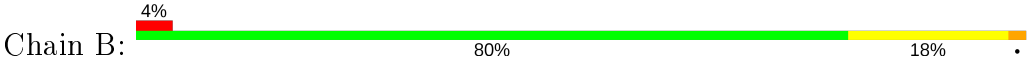
- Molecule 1: Uncharacterized protein

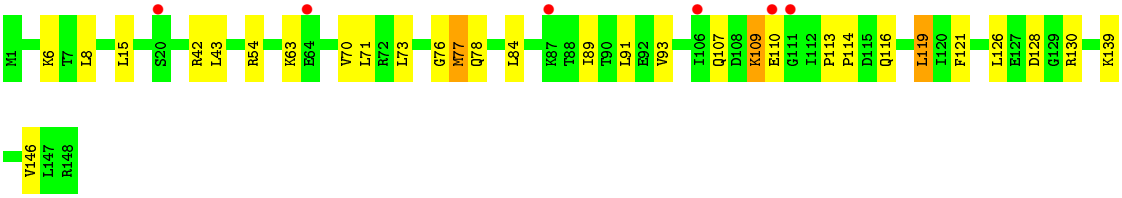
Chain C:



- Molecule 2: Ubiquitin

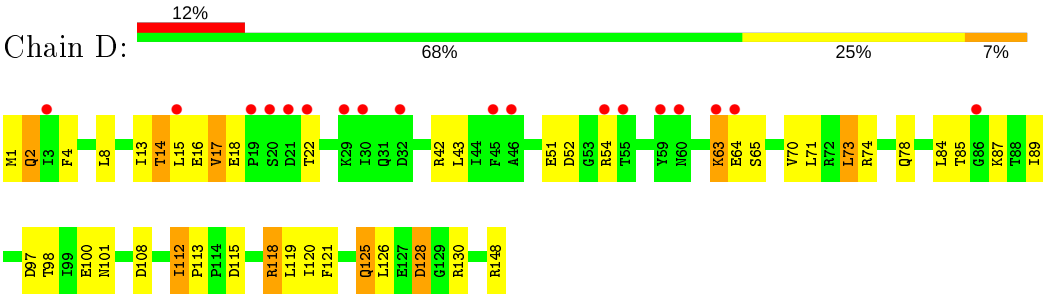
Chain B:





- Molecule 2: Ubiquitin

Chain D:


12%
68%
25%
7%
M1 Q2 I3 F4 L8 I13 T14 L15 E16 V17 E18 P19 S20 D21 T22 K29 I30 Q31 D32 R42 L43 I44 F45 A46 E51 D52 G53 R54 T55 Y59 M60 K63 E64 S65 V70 L71 R72 L73 R74 Q78 L84 T85 G86 K87 T88 I89 T90 L91 E92 V93
D97 T98 I99 E100 N101 D108 I112 P113 P114 D115 R118 L119 I120 F121 Q125 L126 E127 D128 G129 R130 R148

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.63Å 65.37Å 69.85Å 77.66° 89.04° 89.46°	Depositor
Resolution (Å)	49.62 – 2.30 49.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.62-2.30) 97.6 (49.62-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.187 , 0.229 0.191 , 0.228	Depositor DCC
R_{free} test set	1874 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 24.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7358	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.80	0/2478	0.91	7/3338 (0.2%)
1	C	0.78	0/2479	0.93	8/3339 (0.2%)
2	B	0.59	0/1188	0.85	0/1600
2	D	0.61	0/1188	0.78	0/1600
All	All	0.73	0/7333	0.89	15/9877 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	824	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C	824	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	C	611	VAL	CB-CA-C	-6.74	98.59	111.40
1	A	689	LEU	N-CA-C	-6.62	93.12	111.00
1	A	824	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	819	ASP	CB-CG-OD1	6.54	124.19	118.30
1	C	689	LEU	N-CA-C	-6.40	93.73	111.00
1	C	824	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	658	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	C	658	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	753	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	C	819	ASP	CB-CG-OD2	-6.20	112.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	611	VAL	CB-CA-C	-6.08	99.85	111.40
1	A	598	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	753	ARG	NE-CZ-NH1	-5.38	117.61	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	699	SER	Peptide

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	2425	0	2411	41	0
1	C	2426	0	2415	38	0
2	B	1175	0	1226	13	0
2	D	1175	0	1226	31	0
3	C	10	0	0	0	0
4	A	61	0	0	1	0
4	B	12	0	0	0	0
4	C	60	0	0	4	0
4	D	14	0	0	0	0
All	All	7358	0	7278	111	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 8.

All (111) 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)
2:D:98:THR:HG22	2:D:101:ASN:OD1	1.63	0.98
1:C:597:TYR:O	1:C:601:THR:HG23	1.77	0.84
2:D:85:THR:OG1	2:D:87:LYS:HD3	1.77	0.83
1:A:597:TYR:O	1:A:601:THR:HG23	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:SER:O	1:A:675:LYS:NZ	2.17	0.77
1:A:658:ARG:HD2	1:A:670:PHE:O	1.85	0.77
1:C:668:SER:O	1:C:675:LYS:NZ	2.20	0.74
1:A:802:TYR:OH	2:B:73:LEU:O	2.07	0.73
1:C:658:ARG:HD2	1:C:670:PHE:O	1.89	0.73
2:D:1:MET:N	2:D:17:VAL:O	2.22	0.72
2:D:100:GLU:HG3	2:D:128:ASP:HB3	1.75	0.67
1:A:578:GLY:O	1:A:581:VAL:HG12	1.94	0.67
1:C:578:GLY:O	1:C:581:VAL:HG12	1.94	0.66
1:C:597:TYR:O	1:C:601:THR:CG2	2.46	0.64
1:C:592:HIS:HD2	4:C:1017:HOH:O	1.80	0.64
1:A:597:TYR:O	1:A:601:THR:CG2	2.45	0.63
1:A:637:THR:HG22	1:A:638:GLU:HG3	1.79	0.63
1:A:592:HIS:O	1:A:658:ARG:NH2	2.34	0.61
1:C:637:THR:HG22	1:C:638:GLU:HG3	1.83	0.61
2:D:85:THR:OG1	2:D:87:LYS:CD	2.47	0.60
2:D:1:MET:SD	2:D:63:LYS:N	2.75	0.60
1:A:699:SER:O	1:A:702:GLN:HB2	2.02	0.59
1:A:598:LEU:HD13	1:A:680:PHE:CZ	2.39	0.58
1:A:722:VAL:HG13	1:A:854:HIS:HB2	1.86	0.56
1:C:825:ASP:O	1:C:830:GLY:HA3	2.05	0.56
1:C:609:SER:OG	1:C:611:VAL:HG22	2.06	0.56
2:D:93:VAL:HG22	2:D:97:ASP:OD2	2.07	0.55
2:D:16:GLU:O	2:D:17:VAL:HG13	2.06	0.54
2:D:4:PHE:CE1	2:D:14:THR:HG23	2.43	0.54
2:D:22:THR:HG22	2:D:52:ASP:O	2.09	0.53
2:D:14:THR:O	2:D:15:LEU:HD23	2.09	0.53
1:A:633:GLU:O	1:A:637:THR:HB	2.09	0.53
1:A:722:VAL:CG1	1:A:854:HIS:HB2	2.39	0.53
1:C:722:VAL:HG13	1:C:854:HIS:HB2	1.90	0.52
1:A:842:VAL:HG13	1:A:868:LEU:HD22	1.91	0.52
2:D:51:GLU:OE1	2:D:54:ARG:NH1	2.42	0.52
1:C:753:ARG:HD2	4:C:1020:HOH:O	2.11	0.51
1:C:747:LEU:HD22	1:C:789:MET:HE1	1.92	0.51
1:C:598:LEU:HD13	1:C:680:PHE:CZ	2.45	0.51
1:C:859:LYS:HE2	2:D:108:ASP:OD1	2.10	0.51
2:D:16:GLU:HG3	2:D:16:GLU:O	2.10	0.51
1:C:881:THR:HB	4:C:1044:HOH:O	2.11	0.51
1:A:806:VAL:HG13	4:A:928:HOH:O	2.09	0.51
1:A:722:VAL:HG22	1:A:850:PRO:HB3	1.93	0.51
1:A:886:LYS:OXT	1:A:886:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:VAL:HG22	1:C:691:VAL:HG22	1.93	0.51
1:A:609:SER:OG	1:A:611:VAL:HG22	2.09	0.50
1:A:886:LYS:OXT	1:A:886:LYS:CG	2.58	0.50
1:A:858:PRO:HA	1:A:861:ILE:HD12	1.93	0.50
1:C:633:GLU:O	1:C:637:THR:HB	2.12	0.50
1:A:601:THR:HG21	1:A:677:PRO:HB3	1.94	0.50
2:D:112:ILE:HD12	2:D:113:PRO:N	2.26	0.50
1:C:722:VAL:CG1	1:C:854:HIS:HB2	2.42	0.50
2:D:42:ARG:HB2	2:D:70:VAL:HG23	1.94	0.49
1:C:756:LYS:CD	2:D:74:ARG:O	2.60	0.49
1:C:722:VAL:HG22	1:C:850:PRO:HB3	1.95	0.49
1:C:842:VAL:HG13	1:C:868:LEU:HD22	1.95	0.49
1:A:753:ARG:HD3	1:A:759:LYS:HG2	1.95	0.48
1:C:858:PRO:HA	1:C:861:ILE:HD12	1.94	0.48
1:A:676:ASP:OD1	1:A:873:TYR:OH	2.21	0.48
1:C:601:THR:HG21	1:C:677:PRO:HB3	1.95	0.48
1:A:841:GLU:CD	1:A:841:GLU:H	2.17	0.48
1:A:847:LYS:HE3	2:D:148:ARG:HH22	1.80	0.47
1:C:629:LYS:HD3	1:C:633:GLU:OE1	2.14	0.47
1:A:601:THR:HG22	1:A:795:LEU:HD11	1.95	0.47
1:C:601:THR:HG22	1:C:795:LEU:HD11	1.96	0.47
1:A:605:LEU:HD13	1:A:876:MET:SD	2.56	0.46
1:A:629:LYS:HD3	1:A:633:GLU:OE1	2.15	0.46
2:D:100:GLU:CG	2:D:128:ASP:HB3	2.43	0.46
1:A:641:ASN:HB2	1:A:642:PRO:HD3	1.97	0.45
2:D:118:ARG:HD2	2:D:120:ILE:HD11	1.99	0.45
1:A:844:GLU:OE1	2:D:148:ARG:NH2	2.50	0.45
2:B:42:ARG:HB2	2:B:70:VAL:HG23	1.98	0.45
1:C:872:ALA:HB2	4:C:1049:HOH:O	2.16	0.45
2:B:77:MET:HE1	2:B:93:VAL:O	2.17	0.45
1:A:615:VAL:HG22	1:A:691:VAL:HG22	1.99	0.45
1:A:754:PHE:CE1	2:B:71:LEU:HD13	2.52	0.45
1:C:756:LYS:HA	2:D:73:LEU:HD13	1.99	0.44
1:A:801:HIS:HB2	2:B:77:MET:O	2.17	0.44
1:A:615:VAL:HG13	1:A:689:LEU:HD13	1.99	0.44
2:D:118:ARG:HD3	2:D:125:GLN:HG2	1.99	0.44
1:C:760:MET:HG2	1:C:761:PHE:CE2	2.52	0.44
2:D:121:PHE:HB3	2:D:126:LEU:HD21	2.00	0.43
2:B:77:MET:SD	2:B:78:GLN:N	2.91	0.43
1:C:807:LYS:HD2	1:C:815:TRP:CE2	2.53	0.43
1:C:678:GLU:HG3	1:C:709:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:LEU:HD13	1:C:876:MET:SD	2.59	0.43
1:C:754:PHE:CE1	2:D:71:LEU:HD13	2.53	0.43
2:B:121:PHE:HB3	2:B:126:LEU:HD21	2.01	0.43
1:C:756:LYS:HD2	2:D:74:ARG:O	2.19	0.42
1:A:596:SER:OG	2:B:76:GLY:HA2	2.20	0.42
2:B:119:LEU:HA	2:B:119:LEU:HD13	1.85	0.42
2:D:22:THR:CG2	2:D:52:ASP:O	2.68	0.42
2:B:89:ILE:HD11	2:B:109:LYS:HE2	2.00	0.42
2:B:77:MET:SD	2:B:77:MET:C	2.99	0.41
1:C:611:VAL:CG1	1:C:878:GLN:HB2	2.50	0.41
1:C:634:LEU:HD12	1:C:638:GLU:HB2	2.01	0.41
2:D:2:GLN:O	2:D:64:GLU:N	2.31	0.41
1:C:756:LYS:HD3	2:D:74:ARG:O	2.20	0.41
1:A:612:LEU:O	1:A:615:VAL:HB	2.20	0.41
1:A:658:ARG:CD	1:A:670:PHE:O	2.63	0.41
1:A:848:MET:HE2	1:A:848:MET:HB3	1.87	0.41
1:C:615:VAL:HG13	1:C:689:LEU:HD13	2.02	0.41
2:B:107:GLN:HB2	2:B:114:PRO:HD3	2.03	0.41
1:A:611:VAL:CG1	1:A:878:GLN:HB2	2.51	0.41
2:D:112:ILE:HD12	2:D:113:PRO:CD	2.51	0.41
1:A:581:VAL:O	1:A:581:VAL:HG22	2.21	0.41
1:C:753:ARG:HD3	1:C:759:LYS:HG2	2.03	0.41
1:A:807:LYS:HD2	1:A:815:TRP:CE2	2.56	0.40
2:D:13:ILE:HA	2:D:13:ILE:HD13	1.88	0.40
2:B:113:PRO:HA	2:B:114:PRO:HD2	1.89	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	293/312 (94%)	278 (95%)	15 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	293/312 (94%)	278 (95%)	15 (5%)	0	100 100
2	B	146/148 (99%)	139 (95%)	6 (4%)	1 (1%)	22 26
2	D	146/148 (99%)	143 (98%)	3 (2%)	0	100 100
All	All	878/920 (95%)	838 (95%)	39 (4%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	63	LYS

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	271/282 (96%)	244 (90%)	27 (10%)	7 9
1	C	271/282 (96%)	241 (89%)	30 (11%)	6 7
2	B	134/134 (100%)	118 (88%)	16 (12%)	5 5
2	D	134/134 (100%)	113 (84%)	21 (16%)	2 2
All	All	810/832 (97%)	716 (88%)	94 (12%)	5 6

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	LYS
1	A	598	LEU
1	A	601	THR
1	A	605	LEU
1	A	611	VAL
1	A	617	LEU
1	A	625	VAL
1	A	629	LYS
1	A	633	GLU
1	A	635	LEU

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Mol	Chain	Res	Type
1	A	637	THR
1	A	645	ILE
1	A	668	SER
1	A	699	SER
1	A	702	GLN
1	A	703	LYS
1	A	714	MET
1	A	716	LYS
1	A	722	VAL
1	A	736	SER
1	A	756	LYS
1	A	795	LEU
1	A	828	GLN
1	A	851	GLU
1	A	853	LEU
1	A	859	LYS
1	A	886	LYS
2	B	6	LYS
2	B	8	LEU
2	B	15	LEU
2	B	43	LEU
2	B	54	ARG
2	B	77	MET
2	B	84	LEU
2	B	91	LEU
2	B	109	LYS
2	B	110	GLU
2	B	116	GLN
2	B	119	LEU
2	B	128	ASP
2	B	130	ARG
2	B	139	LYS
2	B	146	VAL
1	C	585	LYS
1	C	598	LEU
1	C	601	THR
1	C	605	LEU
1	C	611	VAL
1	C	617	LEU
1	C	621	SER
1	C	625	VAL
1	C	629	LYS

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Mol	Chain	Res	Type
1	C	630	GLU
1	C	633	GLU
1	C	635	LEU
1	C	637	THR
1	C	645	ILE
1	C	668	SER
1	C	675	LYS
1	C	676	ASP
1	C	699	SER
1	C	703	LYS
1	C	714	MET
1	C	722	VAL
1	C	736	SER
1	C	756	LYS
1	C	795	LEU
1	C	810	SER
1	C	851	GLU
1	C	853	LEU
1	C	859	LYS
1	C	866	ARG
1	C	886	LYS
2	D	2	GLN
2	D	8	LEU
2	D	14	THR
2	D	17	VAL
2	D	18	GLU
2	D	43	LEU
2	D	63	LYS
2	D	65	SER
2	D	73	LEU
2	D	78	GLN
2	D	84	LEU
2	D	89	ILE
2	D	91	LEU
2	D	93	VAL
2	D	112	ILE
2	D	115	ASP
2	D	118	ARG
2	D	119	LEU
2	D	125	GLN
2	D	128	ASP
2	D	130	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	138	GLN
1	C	750	GLN
2	D	40	GLN
2	D	125	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	C	902	-	4,4,4	0.58	0	6,6,6	0.73	0
3	SO4	C	901	-	4,4,4	0.49	0	6,6,6	0.72	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 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	299/312 (95%)	-0.51	0 100 100	12, 27, 59, 81	0
1	C	299/312 (95%)	-0.54	1 (0%) 94 96	11, 26, 56, 89	0
2	B	148/148 (100%)	0.15	6 (4%) 37 44	30, 50, 79, 93	0
2	D	148/148 (100%)	0.43	18 (12%) 4 6	26, 55, 94, 111	0
All	All	894/920 (97%)	-0.25	25 (2%) 53 60	11, 33, 78, 111	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	60	ASN	6.9
2	D	3	ILE	4.5
2	D	59	TYR	4.1
2	B	20	SER	3.9
2	D	29	LYS	3.5
2	D	19	PRO	3.3
2	B	87	LYS	3.3
2	D	21	ASP	3.3
2	D	22	THR	3.0
2	D	15	LEU	2.9
1	C	578	GLY	2.9
2	B	106	ILE	2.9
2	D	64	GLU	2.6
2	D	20	SER	2.6
2	D	32	ASP	2.5
2	D	30	ILE	2.5
2	B	64	GLU	2.4
2	D	54	ARG	2.4
2	D	55	THR	2.3
2	B	111	GLY	2.3
2	B	110	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	45	PHE	2.1
2	D	46	ALA	2.1
2	D	63	LYS	2.0
2	D	86	GLY	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	902	5/5	0.95	0.10	47,50,53,56	0
3	SO4	C	901	5/5	0.96	0.13	35,37,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.