Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:39 PM EDT

PDB ID	:	6X1H
Title	:	Crystal structure of a guanine nucleotide exchange factor (GEF) domain from the Orientia tsutsugamushi protein OtDUB
Authors	:	Lim, C.S.; Xiong, Y.
Deposited on	:	2020-05-18
Resolution	:	2.91 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:

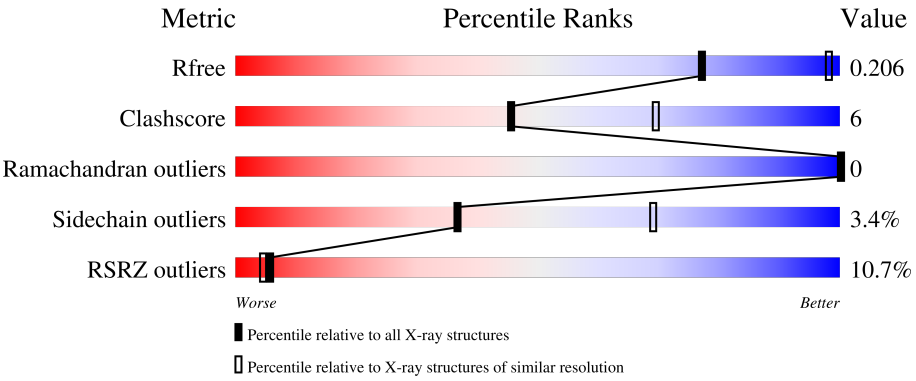
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 <=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	219	21% 76% 19%
1	B	219	10% 85% 11%
1	C	219	18% 84% 12%
1	D	219	2% 79% 18%
1	E	219	3% 84% 14%

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Mol	Chain	Length	Quality of chain
1	F	219	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10290 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 ULP_PROTEASE domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	215	Total	C	N	O	S	0	0	0
			1733	1091	300	338	4			
1	D	216	Total	C	N	O	S	0	0	0
			1743	1097	303	339	4			
1	B	211	Total	C	N	O	S	0	0	0
			1693	1067	288	334	4			
1	F	213	Total	C	N	O	S	0	0	0
			1713	1079	294	336	4			
1	C	213	Total	C	N	O	S	0	0	0
			1713	1079	294	336	4			
1	A	211	Total	C	N	O	S	0	0	0
			1693	1067	288	334	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	547	MET	-	initiating methionine	UNP B3CVM3
E	760	HIS	-	expression tag	UNP B3CVM3
E	761	HIS	-	expression tag	UNP B3CVM3
E	762	HIS	-	expression tag	UNP B3CVM3
E	763	HIS	-	expression tag	UNP B3CVM3
E	764	HIS	-	expression tag	UNP B3CVM3
E	765	HIS	-	expression tag	UNP B3CVM3
D	547	MET	-	initiating methionine	UNP B3CVM3
D	760	HIS	-	expression tag	UNP B3CVM3
D	761	HIS	-	expression tag	UNP B3CVM3
D	762	HIS	-	expression tag	UNP B3CVM3
D	763	HIS	-	expression tag	UNP B3CVM3
D	764	HIS	-	expression tag	UNP B3CVM3
D	765	HIS	-	expression tag	UNP B3CVM3
B	547	MET	-	initiating methionine	UNP B3CVM3
B	760	HIS	-	expression tag	UNP B3CVM3
B	761	HIS	-	expression tag	UNP B3CVM3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	762	HIS	-	expression tag	UNP B3CVM3
B	763	HIS	-	expression tag	UNP B3CVM3
B	764	HIS	-	expression tag	UNP B3CVM3
B	765	HIS	-	expression tag	UNP B3CVM3
F	547	MET	-	initiating methionine	UNP B3CVM3
F	760	HIS	-	expression tag	UNP B3CVM3
F	761	HIS	-	expression tag	UNP B3CVM3
F	762	HIS	-	expression tag	UNP B3CVM3
F	763	HIS	-	expression tag	UNP B3CVM3
F	764	HIS	-	expression tag	UNP B3CVM3
F	765	HIS	-	expression tag	UNP B3CVM3
C	547	MET	-	initiating methionine	UNP B3CVM3
C	760	HIS	-	expression tag	UNP B3CVM3
C	761	HIS	-	expression tag	UNP B3CVM3
C	762	HIS	-	expression tag	UNP B3CVM3
C	763	HIS	-	expression tag	UNP B3CVM3
C	764	HIS	-	expression tag	UNP B3CVM3
C	765	HIS	-	expression tag	UNP B3CVM3
A	547	MET	-	initiating methionine	UNP B3CVM3
A	760	HIS	-	expression tag	UNP B3CVM3
A	761	HIS	-	expression tag	UNP B3CVM3
A	762	HIS	-	expression tag	UNP B3CVM3
A	763	HIS	-	expression tag	UNP B3CVM3
A	764	HIS	-	expression tag	UNP B3CVM3
A	765	HIS	-	expression tag	UNP B3CVM3

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ni 1 1	0	0

- Molecule 3 is water.

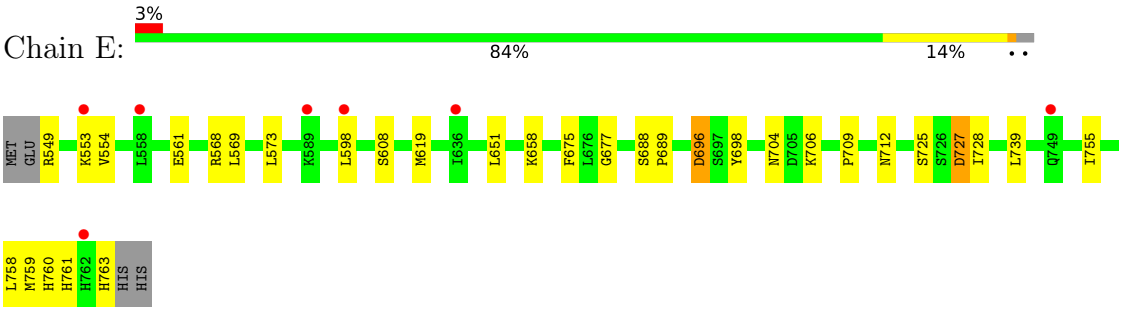
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O 1 1	0	0

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.

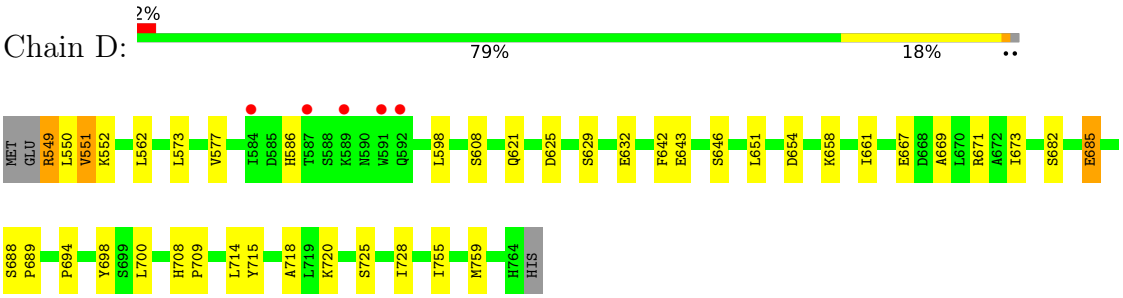
• Molecule 1: ULP_PROTEASE domain-containing protein

Chain E:



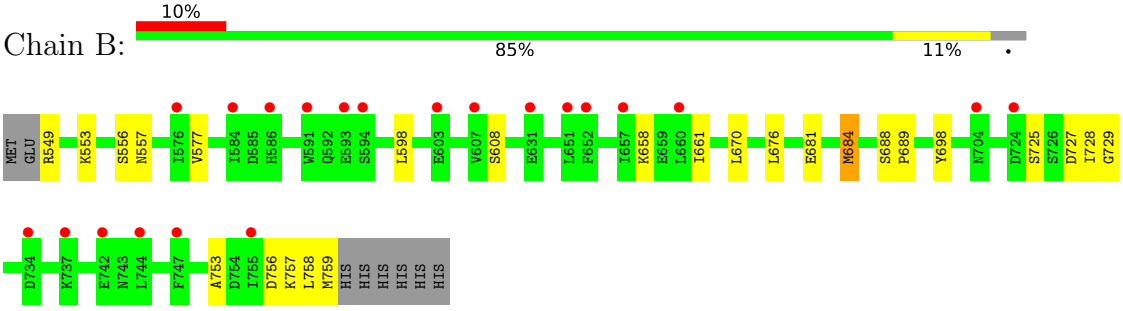
• Molecule 1: ULP_PROTEASE domain-containing protein

Chain D:



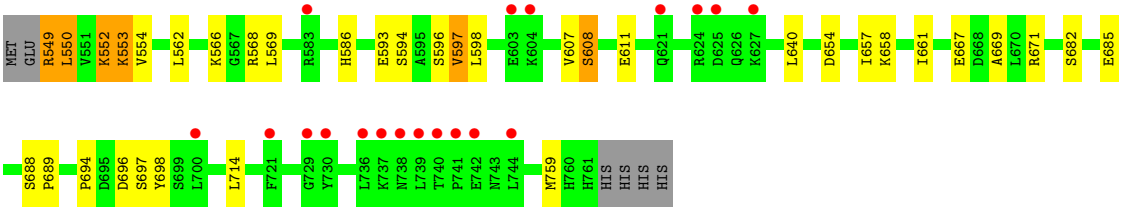
• Molecule 1: ULP_PROTEASE domain-containing protein

Chain B:

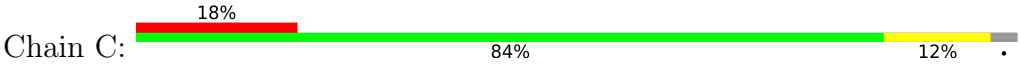


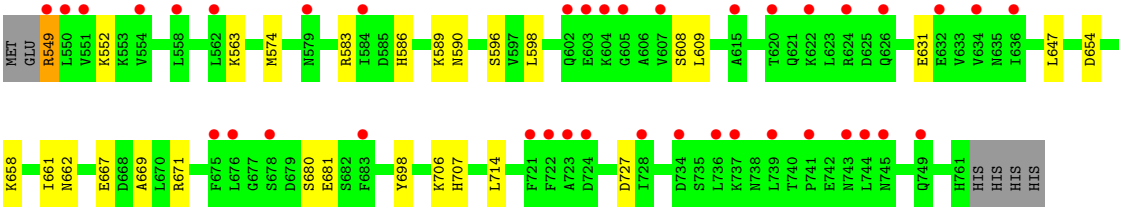
• Molecule 1: ULP_PROTEASE domain-containing protein

Chain F:

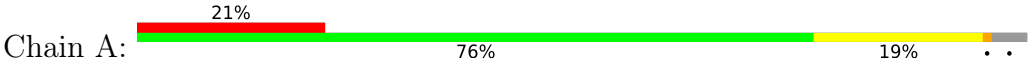


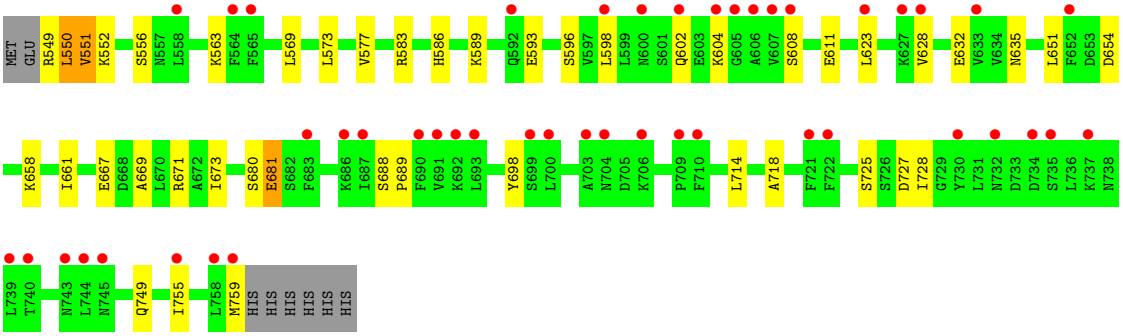
• Molecule 1: ULP_PROTEASE domain-containing protein





• Molecule 1: ULP_PROTEASE domain-containing protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	110.53Å 110.53Å 251.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.86 – 2.91 47.86 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.86-2.91) 99.6 (47.86-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.166 , 0.208 0.171 , 0.206	Depositor DCC
R_{free} test set	1905 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	103.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 88.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.408 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.571 for H, K, L 0.429 for -K, -H, -L	Depositor
Outliers	0 of 37727 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10290	wwPDB-VP
Average B, all atoms (Å^2)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: NI

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	0.75	0/1716	0.84	0/2304
1	B	0.75	0/1716	0.86	0/2304
1	C	0.77	0/1738	0.91	0/2334
1	D	0.83	1/1771 (0.1%)	0.90	0/2379
1	E	0.92	0/1760	0.95	0/2364
1	F	0.82	0/1738	0.89	0/2334
All	All	0.81	1/10439 (0.0%)	0.89	0/14019

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	685	GLU	CD-OE1	7.73	1.34	1.25

There are no bond angle outliers.

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	1693	0	1708	27	0
1	B	1693	0	1708	18	0
1	C	1713	0	1722	11	0
1	D	1743	0	1743	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1733	0	1736	21	3
1	F	1713	0	1722	29	3
2	D	1	0	0	0	0
3	D	1	0	0	0	0
All	All	10290	0	10339	132	3

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 (132) 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:F:550:LEU:H	1:F:550:LEU:HD12	1.01	1.08
1:F:549:ARG:HH21	1:F:549:ARG:HG2	1.32	0.93
1:F:550:LEU:H	1:F:550:LEU:CD1	1.81	0.91
1:F:550:LEU:HD12	1:F:550:LEU:N	1.86	0.88
1:A:550:LEU:N	1:A:550:LEU:HD12	1.90	0.86
1:D:708:HIS:ND1	1:D:709:PRO:HD2	1.93	0.83
1:A:550:LEU:HD12	1:A:550:LEU:H	1.42	0.82
1:E:569:LEU:HD12	1:E:598:LEU:HD13	1.68	0.73
1:D:549:ARG:HG2	1:D:549:ARG:HH11	1.53	0.71
1:F:549:ARG:HG2	1:F:549:ARG:NH2	1.95	0.70
1:D:549:ARG:HG2	1:D:549:ARG:NH1	2.05	0.70
1:A:550:LEU:H	1:A:550:LEU:CD1	2.05	0.69
1:B:670:LEU:HB3	1:B:684:MET:HG2	1.77	0.65
1:F:568:ARG:HG2	1:F:607:VAL:HG11	1.76	0.65
1:E:727:ASP:N	1:E:727:ASP:OD1	2.23	0.65
1:D:549:ARG:HH11	1:D:549:ARG:CG	2.10	0.65
1:B:727:ASP:OD1	1:B:728:ILE:N	2.31	0.63
1:A:550:LEU:N	1:A:550:LEU:CD1	2.61	0.63
1:F:549:ARG:HH21	1:F:549:ARG:CG	2.10	0.60
1:E:706:LYS:HG2	1:D:720:LYS:HA	1.83	0.60
1:A:551:VAL:HG21	1:A:632:GLU:HB3	1.84	0.60
1:C:586:HIS:ND1	1:C:654:ASP:OD1	2.35	0.59
1:B:688:SER:N	1:B:689:PRO:HD2	2.19	0.58
1:F:607:VAL:HG23	1:F:607:VAL:O	2.05	0.57
1:B:549:ARG:N	1:A:681:GLU:OE2	2.39	0.56
1:D:708:HIS:CE1	1:D:709:PRO:HD2	2.40	0.56
1:D:708:HIS:ND1	1:D:709:PRO:CD	2.69	0.54
1:F:694:PRO:HG2	1:F:759:MET:HE2	1.90	0.54
1:A:569:LEU:HD12	1:A:598:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:586:HIS:ND1	1:F:654:ASP:OD1	2.31	0.54
1:D:646:SER:OG	1:B:729:GLY:HA3	2.07	0.53
1:C:669:ALA:HB1	1:C:714:LEU:HD22	1.91	0.52
1:D:577:VAL:HG21	1:D:661:ILE:CD1	2.38	0.52
1:E:739:LEU:O	1:F:596:SER:OG	2.24	0.51
1:E:760:HIS:HA	1:E:763:HIS:CD2	2.45	0.51
1:D:669:ALA:HB1	1:D:714:LEU:HD22	1.91	0.51
1:A:549:ARG:HB2	1:A:550:LEU:HD12	1.92	0.51
1:D:550:LEU:HD12	1:D:550:LEU:O	2.11	0.51
1:B:681:GLU:HA	1:B:684:MET:HE2	1.93	0.51
1:A:632:GLU:O	1:A:635:ASN:HB3	2.11	0.51
1:F:696:ASP:OD1	1:F:759:MET:HE3	2.11	0.50
1:D:694:PRO:HG2	1:D:759:MET:HG3	1.92	0.50
1:E:675:PHE:CE1	1:E:677:GLY:HA3	2.46	0.50
1:A:669:ALA:HB1	1:A:714:LEU:HD22	1.94	0.50
1:F:594:SER:O	1:F:597:VAL:HG13	2.12	0.49
1:C:589:LYS:HG3	1:C:590:ASN:N	2.27	0.49
1:D:755:ILE:O	1:D:759:MET:HG2	2.13	0.49
1:B:549:ARG:N	1:A:681:GLU:CD	2.66	0.49
1:F:593:GLU:O	1:F:597:VAL:HG12	2.13	0.49
1:D:573:LEU:HD11	1:D:651:LEU:HD21	1.95	0.48
1:C:658:LYS:HG2	1:C:698:TYR:CE2	2.48	0.48
1:C:609:LEU:HD22	1:C:647:LEU:HD12	1.96	0.48
1:E:573:LEU:HD11	1:E:651:LEU:HD21	1.96	0.48
1:B:684:MET:HE2	1:B:684:MET:HB2	1.78	0.48
1:F:667:GLU:HB3	1:F:671:ARG:NH1	2.29	0.47
1:E:761:HIS:C	1:E:761:HIS:CD2	2.87	0.47
1:D:673:ILE:HG23	1:D:718:ALA:CB	2.45	0.47
1:A:602:GLN:NE2	1:A:602:GLN:HA	2.28	0.47
1:C:706:LYS:HD2	1:C:707:HIS:CE1	2.50	0.47
1:B:553:LYS:N	1:B:553:LYS:HD3	2.30	0.47
1:F:608:SER:OG	1:F:611:GLU:N	2.44	0.47
1:E:549:ARG:O	1:E:553:LYS:HG3	2.15	0.46
1:A:573:LEU:HD11	1:A:651:LEU:HD21	1.96	0.46
1:C:589:LYS:CG	1:C:590:ASN:N	2.77	0.46
1:F:669:ALA:HB1	1:F:714:LEU:HD22	1.96	0.46
1:F:682:SER:O	1:F:685:GLU:HG3	2.16	0.46
1:D:551:VAL:HG11	1:D:632:GLU:HB3	1.96	0.46
1:B:725:SER:O	1:B:728:ILE:HG22	2.16	0.46
1:E:598:LEU:O	1:E:608:SER:HA	2.16	0.46
1:B:598:LEU:O	1:B:608:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:756:ASP:O	1:B:759:MET:HB3	2.16	0.46
1:F:552:LYS:HA	1:F:552:LYS:HD2	1.62	0.46
1:D:549:ARG:HA	1:D:552:LYS:CD	2.46	0.45
1:F:658:LYS:HG2	1:F:698:TYR:CE2	2.51	0.45
1:D:549:ARG:HA	1:D:552:LYS:HD2	1.97	0.45
1:D:700:LEU:HD23	1:D:700:LEU:N	2.32	0.45
1:E:709:PRO:HB2	1:E:758:LEU:HD21	1.97	0.45
1:A:667:GLU:HB3	1:A:671:ARG:NH1	2.32	0.45
1:D:598:LEU:O	1:D:608:SER:HA	2.16	0.45
1:F:697:SER:HA	1:F:759:MET:HE1	1.99	0.45
1:A:552:LYS:HE2	1:A:552:LYS:HB3	1.82	0.45
1:A:586:HIS:ND1	1:A:654:ASP:OD1	2.32	0.44
1:A:658:LYS:HG2	1:A:698:TYR:CE2	2.52	0.44
1:E:573:LEU:HD11	1:E:651:LEU:CD2	2.47	0.44
1:C:598:LEU:O	1:C:608:SER:HA	2.18	0.44
1:A:725:SER:O	1:A:728:ILE:HG22	2.18	0.44
1:D:586:HIS:HD2	1:D:654:ASP:OD1	2.00	0.44
1:F:688:SER:HB3	1:F:689:PRO:HD3	2.00	0.44
1:A:598:LEU:O	1:A:608:SER:HA	2.17	0.44
1:E:658:LYS:HG2	1:E:698:TYR:CE2	2.53	0.43
1:D:651:LEU:HD23	1:D:651:LEU:HA	1.83	0.43
1:D:658:LYS:HG2	1:D:698:TYR:CE2	2.53	0.43
1:D:688:SER:HB3	1:D:689:PRO:HD3	2.00	0.43
1:E:696:ASP:OD1	1:E:696:ASP:N	2.48	0.43
1:F:569:LEU:CD1	1:F:598:LEU:HD13	2.49	0.43
1:E:651:LEU:HD23	1:E:651:LEU:HA	1.85	0.43
1:E:688:SER:HB3	1:E:689:PRO:HD3	2.00	0.43
1:F:568:ARG:HG2	1:F:607:VAL:CG1	2.47	0.43
1:D:562:LEU:HD13	1:D:643:GLU:HG3	2.01	0.43
1:D:700:LEU:HD11	1:D:759:MET:SD	2.58	0.43
1:A:755:ILE:O	1:A:759:MET:HG2	2.19	0.43
1:D:586:HIS:CD2	1:D:654:ASP:OD1	2.71	0.43
1:B:553:LYS:N	1:B:553:LYS:CD	2.80	0.43
1:A:623:LEU:O	1:A:628:VAL:HG23	2.18	0.43
1:F:657:ILE:O	1:F:661:ILE:HG12	2.19	0.42
1:E:554:VAL:HG13	1:E:619:MET:SD	2.59	0.42
1:D:725:SER:O	1:D:728:ILE:HG22	2.20	0.42
1:E:688:SER:N	1:E:689:PRO:CD	2.83	0.42
1:F:640:LEU:HD12	1:F:640:LEU:HA	1.83	0.42
1:E:704:ASN:O	1:D:720:LYS:NZ	2.53	0.42
1:C:661:ILE:HG23	1:C:662:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:LYS:HD3	1:A:563:LYS:HA	1.74	0.42
1:B:658:LYS:HG2	1:B:698:TYR:CE2	2.54	0.42
1:B:753:ALA:O	1:B:757:LYS:HG3	2.19	0.42
1:A:688:SER:HB3	1:A:689:PRO:HD3	2.01	0.42
1:A:577:VAL:HG21	1:A:661:ILE:CD1	2.50	0.42
1:C:667:GLU:HB3	1:C:671:ARG:NH1	2.35	0.41
1:C:549:ARG:CG	1:C:552:LYS:HD2	2.51	0.41
1:B:577:VAL:HG21	1:B:661:ILE:CD1	2.50	0.41
1:F:550:LEU:O	1:F:554:VAL:HG23	2.20	0.41
1:E:755:ILE:O	1:E:759:MET:HG2	2.21	0.41
1:F:562:LEU:O	1:F:566:LYS:HG3	2.20	0.41
1:D:621:GLN:NE2	1:D:625:ASP:OD1	2.53	0.41
1:A:651:LEU:HD23	1:A:651:LEU:HA	1.86	0.41
1:E:712:ASN:ND2	1:D:715:TYR:CD2	2.89	0.41
1:D:667:GLU:O	1:D:671:ARG:HG3	2.21	0.41
1:D:682:SER:HA	1:D:685:GLU:HG2	2.02	0.41
1:B:758:LEU:HD12	1:B:758:LEU:HA	1.85	0.41
1:D:642:PHE:CZ	1:B:676:LEU:HD21	2.56	0.40
1:F:598:LEU:O	1:F:608:SER:HA	2.20	0.40
1:A:673:ILE:HG23	1:A:718:ALA:CB	2.52	0.40
1:A:573:LEU:HD11	1:A:651:LEU:CD2	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:561:GLU:OE1	1:F:553:LYS:NZ[3_455]	1.57	0.63
1:E:561:GLU:CD	1:F:553:LYS:NZ[3_455]	1.64	0.56
1:E:561:GLU:OE2	1:F:553:LYS:NZ[3_455]	1.72	0.48

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	209/219 (95%)	206 (99%)	3 (1%)	0	100	100
1	B	209/219 (95%)	207 (99%)	2 (1%)	0	100	100
1	C	211/219 (96%)	209 (99%)	2 (1%)	0	100	100
1	D	214/219 (98%)	211 (99%)	3 (1%)	0	100	100
1	E	213/219 (97%)	210 (99%)	3 (1%)	0	100	100
1	F	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
All	All	1267/1314 (96%)	1251 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	191/199 (96%)	178 (93%)	13 (7%)	16	40
1	B	191/199 (96%)	188 (98%)	3 (2%)	62	85
1	C	193/199 (97%)	184 (95%)	9 (5%)	26	58
1	D	196/199 (98%)	193 (98%)	3 (2%)	65	86
1	E	195/199 (98%)	190 (97%)	5 (3%)	46	76
1	F	193/199 (97%)	187 (97%)	6 (3%)	40	72
All	All	1159/1194 (97%)	1120 (97%)	39 (3%)	37	69

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	568	ARG
1	E	696	ASP
1	E	725	SER
1	E	727	ASP
1	E	728	ILE
1	D	549	ARG
1	D	551	VAL

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Mol	Chain	Res	Type
1	D	629	SER
1	B	556	SER
1	B	557	ASN
1	B	684	MET
1	F	549	ARG
1	F	550	LEU
1	F	552	LYS
1	F	553	LYS
1	F	597	VAL
1	F	608	SER
1	C	549	ARG
1	C	563	LYS
1	C	574	MET
1	C	583	ARG
1	C	596	SER
1	C	631	GLU
1	C	680	SER
1	C	681	GLU
1	C	727	ASP
1	A	550	LEU
1	A	551	VAL
1	A	556	SER
1	A	583	ARG
1	A	589	LYS
1	A	593	GLU
1	A	596	SER
1	A	604	LYS
1	A	611	GLU
1	A	680	SER
1	A	681	GLU
1	A	727	ASP
1	A	749	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	761	HIS
1	E	762	HIS
1	D	586	HIS
1	D	761	HIS
1	B	557	ASN
1	B	707	HIS

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Mol	Chain	Res	Type
1	A	602	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	211/219 (96%)	0.94	46 (21%) 0 0	119, 185, 241, 288	0
1	B	211/219 (96%)	0.57	21 (9%) 7 5	123, 175, 212, 254	0
1	C	213/219 (97%)	0.90	39 (18%) 1 1	109, 170, 243, 277	0
1	D	216/219 (98%)	0.17	5 (2%) 60 59	81, 127, 185, 209	0
1	E	215/219 (98%)	0.33	7 (3%) 46 42	70, 118, 168, 197	0
1	F	213/219 (97%)	0.52	19 (8%) 9 7	79, 139, 191, 223	0
All	All	1279/1314 (97%)	0.57	137 (10%) 6 4	70, 152, 223, 288	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	744	LEU	9.6
1	A	607	VAL	5.8
1	C	604	LYS	5.6
1	F	742	GLU	5.5
1	C	626	GLN	5.3
1	C	724	ASP	5.2
1	C	551	VAL	5.1
1	F	739	LEU	4.9
1	C	737	LYS	4.9
1	A	734	ASP	4.7
1	B	737	LYS	4.7
1	C	602	GLN	4.7
1	C	678	SER	4.6
1	A	759	MET	4.6
1	A	628	VAL	4.5
1	F	740	THR	4.5
1	B	734	ASP	4.5
1	A	704	ASN	4.4
1	C	749	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	624	ARG	4.2
1	A	700	LEU	4.1
1	C	603	GLU	4.0
1	C	558	LEU	4.0
1	A	755	ILE	3.9
1	A	605	GLY	3.9
1	C	636	ILE	3.8
1	F	604	LYS	3.8
1	C	744	LEU	3.8
1	A	743	ASN	3.6
1	F	744	LEU	3.6
1	A	604	LYS	3.6
1	F	737	LYS	3.5
1	A	592	GLN	3.4
1	A	732	ASN	3.4
1	B	652	PHE	3.4
1	A	598	LEU	3.4
1	A	693	LEU	3.4
1	C	622	LYS	3.4
1	C	549	ARG	3.3
1	A	739	LEU	3.3
1	A	627	LYS	3.2
1	B	724	ASP	3.2
1	C	743	ASN	3.2
1	A	735	SER	3.2
1	B	607	VAL	3.2
1	C	607	VAL	3.2
1	A	699	SER	3.1
1	C	676	LEU	3.1
1	A	691	VAL	3.1
1	C	550	LEU	3.1
1	A	606	ALA	3.1
1	B	576	ILE	3.1
1	B	584	ILE	3.0
1	A	608	SER	3.0
1	A	758	LEU	3.0
1	A	721	PHE	3.0
1	F	603	GLU	3.0
1	F	730	TYR	2.9
1	D	592	GLN	2.9
1	D	589	LYS	2.9
1	C	683	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	703	ALA	2.9
1	B	651	LEU	2.9
1	A	710	PHE	2.9
1	B	744	LEU	2.9
1	A	737	LYS	2.9
1	F	738	ASN	2.8
1	A	558	LEU	2.8
1	D	591	TRP	2.8
1	C	723	ALA	2.8
1	A	745	ASN	2.8
1	E	762	HIS	2.8
1	C	736	LEU	2.8
1	B	742	GLU	2.8
1	F	624	ARG	2.8
1	F	621	GLN	2.8
1	C	745	ASN	2.7
1	C	739	LEU	2.7
1	C	634	VAL	2.7
1	B	747	PHE	2.7
1	C	675	PHE	2.6
1	C	620	THR	2.6
1	E	558	LEU	2.6
1	A	730	TYR	2.6
1	B	657	ILE	2.6
1	F	583	ARG	2.6
1	B	755	ILE	2.6
1	C	734	ASP	2.6
1	B	591	TRP	2.6
1	C	722	PHE	2.5
1	F	736	LEU	2.5
1	A	602	GLN	2.5
1	D	587	THR	2.5
1	A	652	PHE	2.5
1	A	623	LEU	2.5
1	A	692	LYS	2.4
1	A	683	PHE	2.4
1	B	586	HIS	2.4
1	E	589	LYS	2.4
1	F	625	ASP	2.4
1	B	704	ASN	2.4
1	C	554	VAL	2.4
1	A	706	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	749	GLN	2.3
1	E	598	LEU	2.3
1	C	741	PRO	2.3
1	A	564	PHE	2.3
1	A	633	VAL	2.3
1	A	740	THR	2.3
1	B	660	LEU	2.3
1	C	562	LEU	2.2
1	A	565	PHE	2.2
1	D	584	ILE	2.2
1	C	605	GLY	2.2
1	B	603	GLU	2.2
1	B	631	GLU	2.2
1	A	687	ILE	2.2
1	A	686	LYS	2.2
1	F	729	GLY	2.2
1	E	636	ILE	2.2
1	C	728	ILE	2.2
1	F	721	PHE	2.1
1	E	553	LYS	2.1
1	A	690	PHE	2.1
1	C	615	ALA	2.1
1	A	600	ASN	2.1
1	B	593	GLU	2.1
1	C	632	GLU	2.1
1	A	722	PHE	2.1
1	C	584	ILE	2.1
1	C	579	ASN	2.1
1	B	594	SER	2.1
1	A	709	PRO	2.1
1	C	721	PHE	2.1
1	F	627	LYS	2.0
1	F	741	PRO	2.0
1	F	700	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)

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
2	NI	D	801	1/1	0.94	0.19	87,87,87,87	1

6.5 Other polymers (i)

There are no such residues in this entry.