wwPDB X-ray Structure Validation Summary Report (i)

Mar 22, 2025 – 02:53 PM EDT

PDB ID	:	4DHJ
Title	:	The structure of a ceOTUB1 ubiquitin aldehyde UBC13 Ub complex
Authors	:	Wiener, R.; Zhang, X.; Wang, T.; Wolberger, C.
Deposited on	:	2012-01-27
Resolution	:	2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

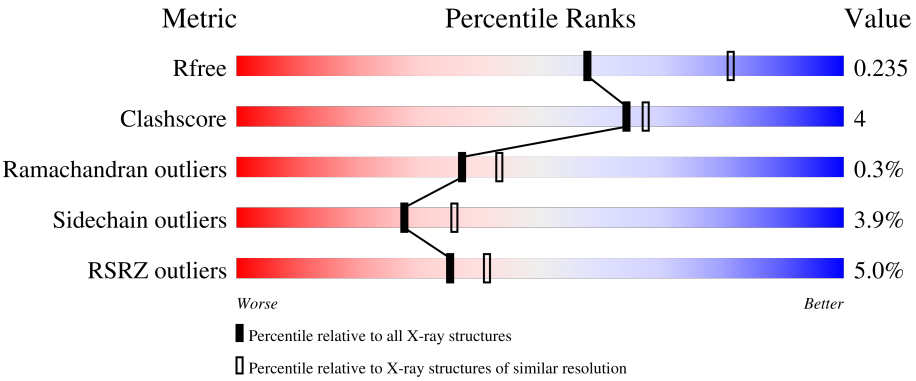
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	284	2% 79% 8% 13%
1	E	284	3% 75% 10% 14%
1	I	284	% 75% 9% 15%
1	L	284	% 75% 9% 16%
2	B	76	% 86% 14%

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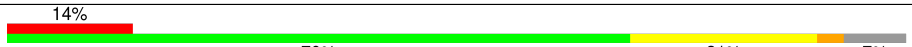
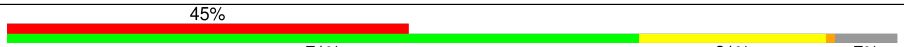
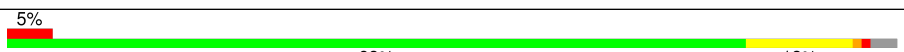
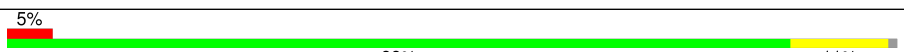
Mol	Chain	Length	Quality of chain
2	F	76	
2	J	76	
2	M	76	
3	D	76	
3	H	76	
4	C	152	
4	G	152	
4	K	152	
4	N	152	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16392 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 Ubiquitin thioesterase otubain-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	1	0
			2013	1288	327	388	10			
1	E	245	Total	C	N	O	S	0	0	0
			1968	1260	317	381	10			
1	I	241	Total	C	N	O	S	0	0	0
			1942	1244	314	374	10			
1	L	239	Total	C	N	O	S	0	0	0
			1921	1233	312	366	10			

- Molecule 2 is a protein called Ubiquitin aldehyde.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	F	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	J	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	M	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	71	Total	C	N	O	S	0	0	0
			563	356	94	112	1			
3	H	71	Total	C	N	O	S	0	0	0
			559	353	93	112	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	576	CYS	GLY	engineered mutation	UNP P0CG48
H	576	CYS	GLY	engineered mutation	UNP P0CG48

- Molecule 4 is a protein called Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	149	Total	C	N	O	S	0	1	0
			1185	759	204	218	4			
4	K	148	Total	C	N	O	S	0	0	0
			1171	751	202	214	4			
4	G	148	Total	C	N	O	S	0	0	0
			1174	754	202	214	4			
4	N	150	Total	C	N	O	S	0	0	0
			1187	762	206	215	4			

- Molecule 5 is water.

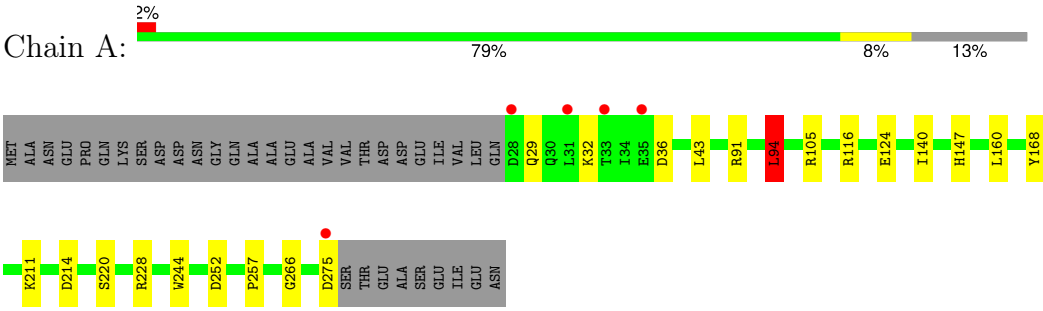
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		
5	B	21	Total	O	0	0
			21	21		
5	E	30	Total	O	0	0
			30	30		
5	F	2	Total	O	0	0
			2	2		
5	D	5	Total	O	0	0
			5	5		
5	C	34	Total	O	0	0
			34	34		
5	I	35	Total	O	0	0
			35	35		
5	J	9	Total	O	0	0
			9	9		
5	K	5	Total	O	0	0
			5	5		
5	G	17	Total	O	0	0
			17	17		
5	L	53	Total	O	0	0
			53	53		
5	M	10	Total	O	0	0
			10	10		
5	N	30	Total	O	0	0
			30	30		

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.

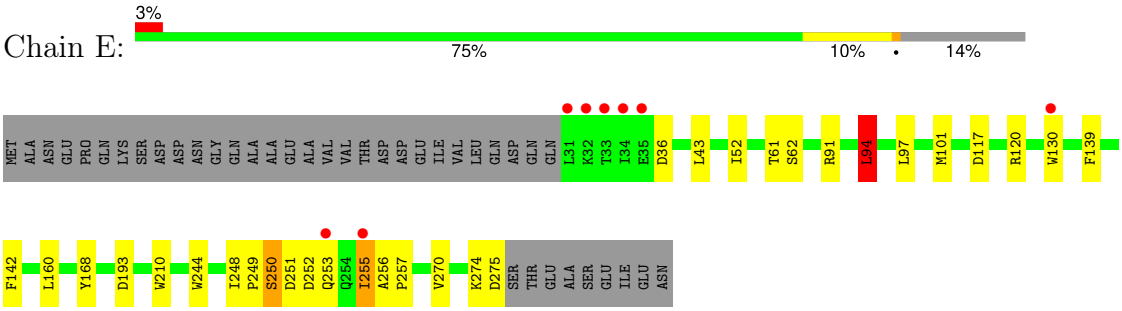
• Molecule 1: Ubiquitin thioesterase otubain-like

Chain A:



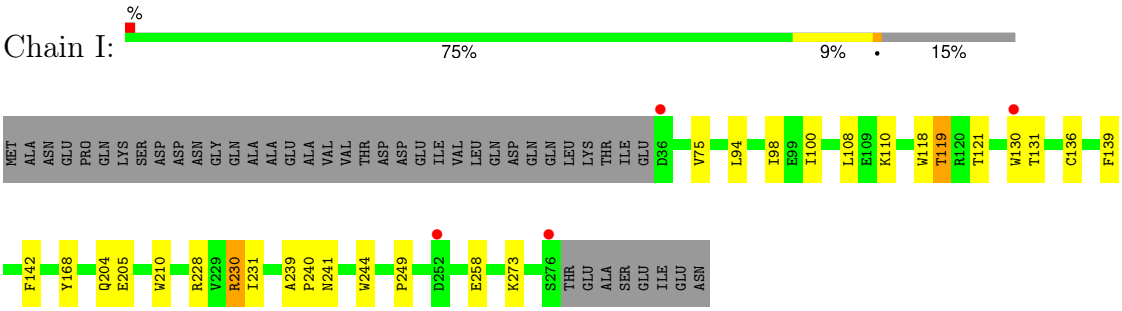
• Molecule 1: Ubiquitin thioesterase otubain-like

Chain E:



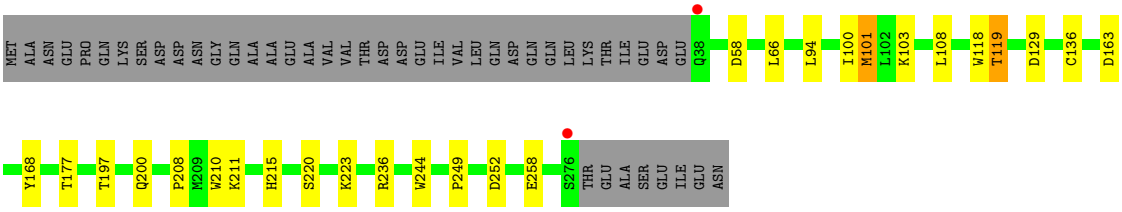
• Molecule 1: Ubiquitin thioesterase otubain-like

Chain I:

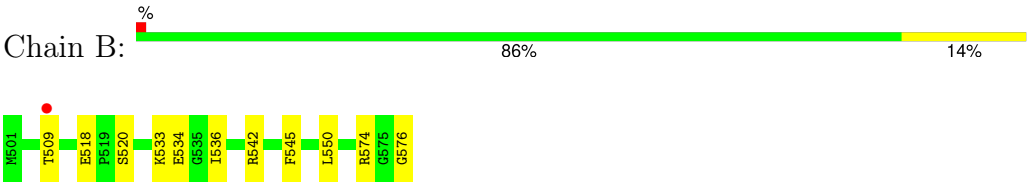


• Molecule 1: Ubiquitin thioesterase otubain-like

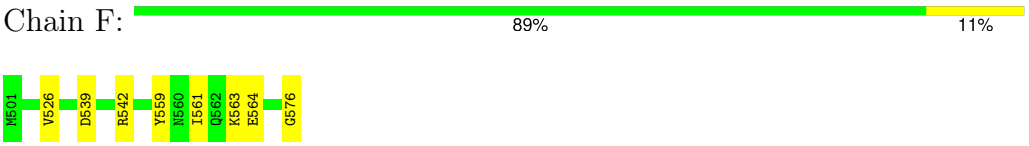
Chain L:



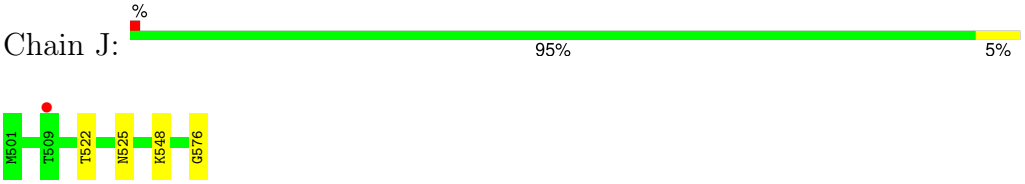
• Molecule 2: Ubiquitin aldehyde



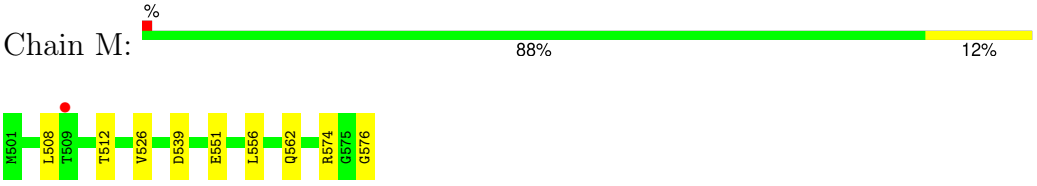
• Molecule 2: Ubiquitin aldehyde



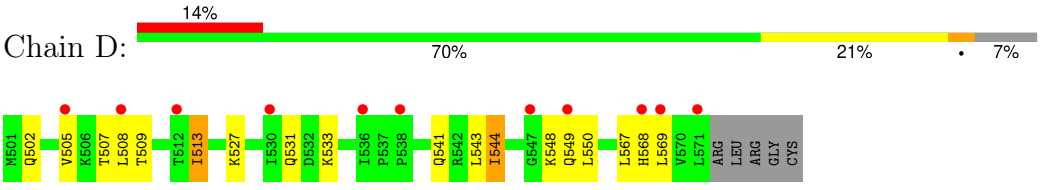
• Molecule 2: Ubiquitin aldehyde



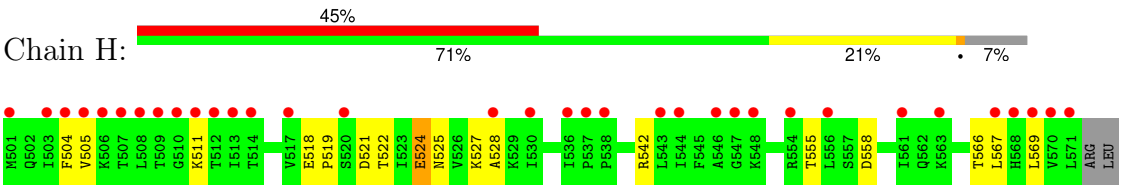
• Molecule 2: Ubiquitin aldehyde



• Molecule 3: Ubiquitin

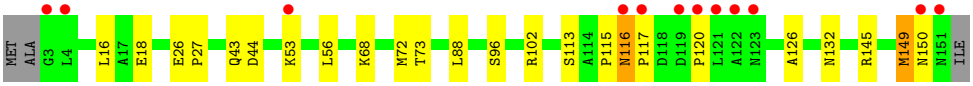


• Molecule 3: Ubiquitin



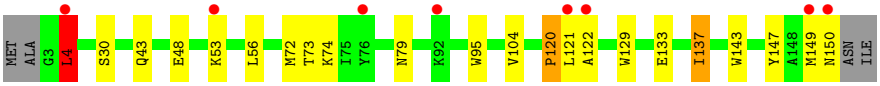
• Molecule 4: Ubiquitin-conjugating enzyme E2 N

Chain C:



• Molecule 4: Ubiquitin-conjugating enzyme E2 N

Chain K:

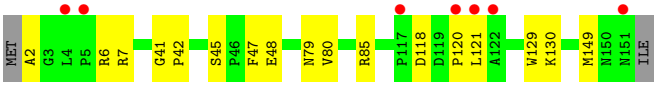


• Molecule 4: Ubiquitin-conjugating enzyme E2 N

Chain G:

• Molecule 4: Ubiquitin-conjugating enzyme E2 N

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.45Å 182.81Å 242.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.67 – 2.35 39.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.67-2.35) 99.7 (39.67-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.237 0.201 , 0.235	Depositor DCC
R_{free} test set	6452 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16392	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: GLZ

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	0.65	1/2063 (0.0%)	0.70	1/2798 (0.0%)
1	E	0.57	2/2015 (0.1%)	0.66	1/2737 (0.0%)
1	I	0.63	3/1989 (0.2%)	0.67	0/2699
1	L	0.64	3/1968 (0.2%)	0.67	0/2671
2	B	0.54	0/599	0.69	0/806
2	F	0.47	0/603	0.64	0/811
2	J	0.50	0/603	0.66	0/811
2	M	0.56	0/603	0.71	0/811
3	D	0.41	0/569	0.63	0/767
3	H	0.42	0/565	0.68	1/763 (0.1%)
4	C	0.60	0/1218	0.74	0/1660
4	G	0.56	2/1204 (0.2%)	0.64	0/1641
4	K	0.56	2/1201 (0.2%)	0.67	1/1637 (0.1%)
4	N	0.60	1/1217 (0.1%)	0.71	0/1658
All	All	0.58	14/16417 (0.1%)	0.68	4/22270 (0.0%)

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	E	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	244	TRP	CD2-CE2	6.05	1.48	1.41
1	I	210	TRP	CD2-CE2	6.05	1.48	1.41
4	K	129	TRP	CD2-CE2	6.00	1.48	1.41
4	N	129	TRP	CD2-CE2	5.91	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	210	TRP	CD2-CE2	5.75	1.48	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	558	ASP	CB-CG-OD1	8.81	126.23	118.30
1	E	94	LEU	CA-CB-CG	7.43	132.39	115.30
1	A	94	LEU	CA-CB-CG	7.00	131.41	115.30
4	K	4	LEU	CA-CB-CG	5.75	128.52	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	250	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	2013	0	1944	13	0
1	E	1968	0	1880	13	0
1	I	1942	0	1864	13	0
1	L	1921	0	1850	15	0
2	B	597	0	619	7	0
2	F	601	0	625	3	0
2	J	601	0	625	1	0
2	M	601	0	625	3	0
3	D	563	0	583	9	0
3	H	559	0	572	6	0
4	C	1185	0	1183	13	0
4	G	1174	0	1180	11	0
4	K	1171	0	1171	12	0
4	N	1187	0	1198	9	0
5	A	58	0	0	5	0
5	B	21	0	0	4	0
5	C	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	5	0	0	0	0
5	E	30	0	0	0	0
5	F	2	0	0	0	0
5	G	17	0	0	0	0
5	I	35	0	0	0	0
5	J	9	0	0	0	0
5	K	5	0	0	0	0
5	L	53	0	0	1	0
5	M	10	0	0	1	0
5	N	30	0	0	0	0
All	All	16392	0	15919	120	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 4.

The worst 5 of 120 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)
4:N:45:SER:O	4:N:48:GLU:OE1	1.96	0.84
1:L:197:THR:HG23	1:L:200:GLN:H	1.44	0.82
4:N:42:PRO:O	4:N:48:GLU:OE2	1.97	0.81
1:A:193:ASP:OD2	2:B:542:ARG:NH2	2.17	0.78
4:K:133:GLU:O	4:K:137:ILE:HG22	1.86	0.75

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	247/284 (87%)	236 (96%)	11 (4%)	0	100	100
1	E	243/284 (86%)	235 (97%)	6 (2%)	2 (1%)	16	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	239/284 (84%)	233 (98%)	6 (2%)	0	100 100
1	L	237/284 (84%)	230 (97%)	6 (2%)	1 (0%)	30 34
2	B	74/76 (97%)	74 (100%)	0	0	100 100
2	F	74/76 (97%)	74 (100%)	0	0	100 100
2	J	74/76 (97%)	72 (97%)	2 (3%)	0	100 100
2	M	74/76 (97%)	72 (97%)	2 (3%)	0	100 100
3	D	69/76 (91%)	67 (97%)	2 (3%)	0	100 100
3	H	69/76 (91%)	64 (93%)	5 (7%)	0	100 100
4	C	148/152 (97%)	138 (93%)	10 (7%)	0	100 100
4	G	146/152 (96%)	141 (97%)	5 (3%)	0	100 100
4	K	146/152 (96%)	136 (93%)	8 (6%)	2 (1%)	9 7
4	N	148/152 (97%)	144 (97%)	4 (3%)	0	100 100
All	All	1988/2200 (90%)	1916 (96%)	67 (3%)	5 (0%)	37 43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	252	ASP
1	E	253	GLN
4	K	121	LEU
1	E	252	ASP
4	K	120	PRO

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	216/245 (88%)	210 (97%)	6 (3%)	38 49
1	E	209/245 (85%)	201 (96%)	8 (4%)	28 37
1	I	207/245 (84%)	201 (97%)	6 (3%)	37 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	204/245 (83%)	198 (97%)	6 (3%)	37 48
2	B	67/68 (98%)	64 (96%)	3 (4%)	23 29
2	F	68/68 (100%)	66 (97%)	2 (3%)	37 48
2	J	68/68 (100%)	67 (98%)	1 (2%)	60 73
2	M	68/68 (100%)	64 (94%)	4 (6%)	16 18
3	D	65/69 (94%)	58 (89%)	7 (11%)	5 5
3	H	64/69 (93%)	59 (92%)	5 (8%)	10 10
4	C	126/129 (98%)	118 (94%)	8 (6%)	15 16
4	G	125/129 (97%)	120 (96%)	5 (4%)	27 34
4	K	124/129 (96%)	120 (97%)	4 (3%)	34 43
4	N	126/129 (98%)	124 (98%)	2 (2%)	58 71
All	All	1737/1906 (91%)	1670 (96%)	67 (4%)	27 36

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	539	ASP
2	M	574	ARG
4	N	121	LEU
3	D	544	ILE
3	D	533	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	147	HIS
2	M	502	GLN
2	M	525	ASN
2	F	525	ASN
2	F	549	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	GLZ	J	576	2,1	3,3,3	2.11	1 (33%)	1,2,2	1.30	0
2	GLZ	F	576	2,1	3,3,3	2.42	1 (33%)	1,2,2	0.85	0
2	GLZ	M	576	2,1	3,3,3	2.28	1 (33%)	1,2,2	1.87	0
2	GLZ	B	576	2,1	3,3,3	2.02	1 (33%)	1,2,2	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLZ	J	576	2,1	-	0/0/1/1	-
2	GLZ	F	576	2,1	-	0/0/1/1	-
2	GLZ	M	576	2,1	-	0/0/1/1	-
2	GLZ	B	576	2,1	-	0/0/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	576	GLZ	O-C	4.13	1.43	1.20
2	M	576	GLZ	O-C	3.89	1.42	1.20
2	J	576	GLZ	O-C	3.61	1.40	1.20
2	B	576	GLZ	O-C	3.44	1.39	1.20

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.

5.5 Carbohydrates (i)

There are no oligosaccharides 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	248/284 (87%)	-0.30	5 (2%) 64 69	32, 45, 88, 143	1 (0%)
1	E	245/284 (86%)	-0.09	8 (3%) 49 55	39, 54, 103, 137	0
1	I	241/284 (84%)	-0.22	4 (1%) 69 73	34, 51, 83, 122	0
1	L	239/284 (84%)	-0.31	2 (0%) 82 85	30, 46, 80, 120	0
2	B	75/76 (98%)	-0.17	1 (1%) 74 79	36, 50, 71, 77	0
2	F	75/76 (98%)	-0.07	0 100 100	44, 65, 94, 104	0
2	J	75/76 (98%)	-0.16	1 (1%) 74 79	41, 58, 85, 93	0
2	M	75/76 (98%)	-0.31	1 (1%) 74 79	35, 50, 67, 78	0
3	D	71/76 (93%)	1.08	11 (15%) 6 7	57, 108, 154, 159	0
3	H	71/76 (93%)	2.04	34 (47%) 0 0	102, 153, 185, 196	0
4	C	149/152 (98%)	0.07	12 (8%) 19 23	31, 49, 103, 145	1 (0%)
4	G	148/152 (97%)	0.36	7 (4%) 37 43	50, 67, 111, 145	0
4	K	148/152 (97%)	0.37	8 (5%) 32 37	50, 67, 108, 142	0
4	N	150/152 (98%)	0.06	7 (4%) 37 43	36, 54, 103, 143	0
All	All	2010/2200 (91%)	0.04	101 (5%) 35 41	30, 56, 130, 196	2 (0%)

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	121	LEU	5.9
3	D	547	GLY	5.9
3	H	508	LEU	5.8
1	E	31	LEU	5.7
3	D	571	LEU	5.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	GLZ	F	576	4/4	0.90	0.13	61,64,67,71	0
2	GLZ	B	576	4/4	0.94	0.12	50,54,57,63	0
2	GLZ	J	576	4/4	0.96	0.08	50,53,54,54	0
2	GLZ	M	576	4/4	0.96	0.07	44,47,50,52	0

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.