



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2017 – 01:08 AM 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 : unknown
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

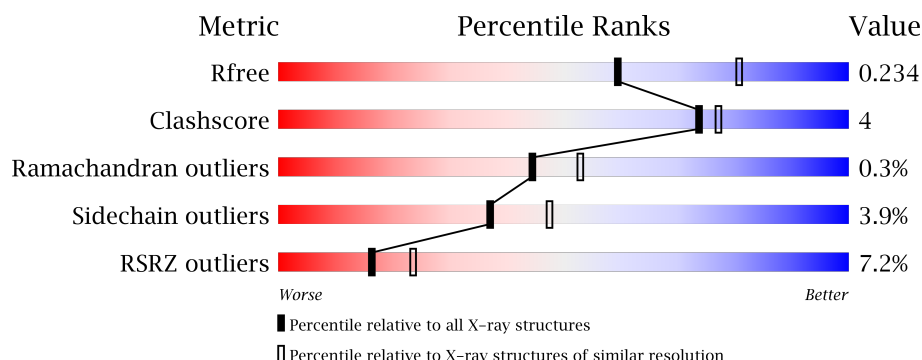
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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. 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 $\leq 5\%$. 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	<div> <div>2%</div> <div>79% 8% 13%</div> </div>
1	E	284	<div> <div>2%</div> <div>75% 10% 14%</div> </div>
1	I	284	<div> <div>2%</div> <div>75% 9% 15%</div> </div>
1	L	284	<div> <div>0%</div> <div>75% 9% 16%</div> </div>
2	B	76	<div> <div>3%</div> <div>87% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	76	<div><div></div><div>3%</div><div>91%</div><div>9%</div></div>
2	J	76	<div><div></div><div>%</div><div>96%</div><div></div><div>.</div></div>
2	M	76	<div><div></div><div>89%</div><div>11%</div></div>
3	D	76	<div><div></div><div>39%</div><div>70%</div><div>21%</div><div>.</div><div>7%</div></div>
3	H	76	<div><div></div><div>62%</div><div>71%</div><div>21%</div><div>.</div><div>7%</div></div>
4	C	152	<div><div></div><div>8%</div><div>82%</div><div>14%</div><div>..</div></div>
4	G	152	<div><div></div><div>9%</div><div>82%</div><div>15%</div><div>..</div></div>
4	K	152	<div><div></div><div>3%</div><div>83%</div><div>13%</div><div>..</div><div>.</div></div>
4	N	152	<div><div></div><div>5%</div><div>88%</div><div>11%</div><div>.</div></div>

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			

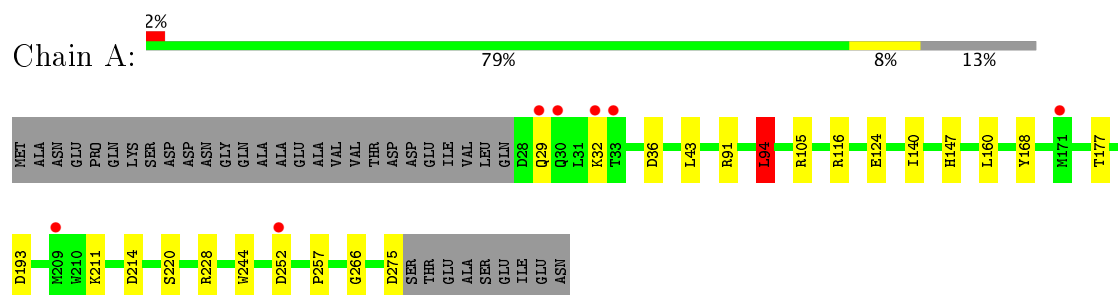
- Molecule 5 is water.

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		

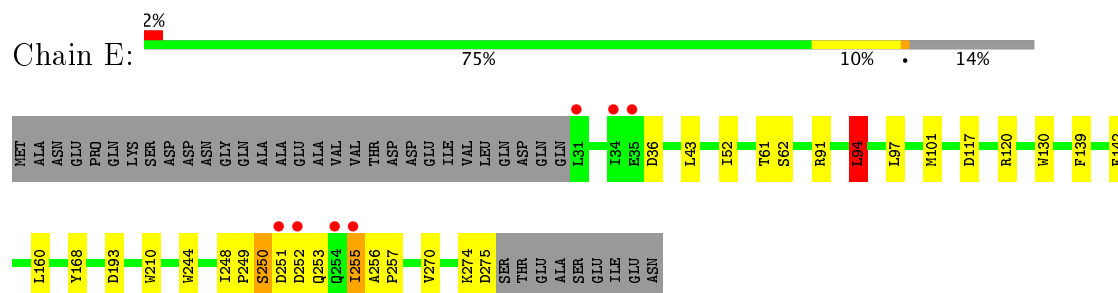
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

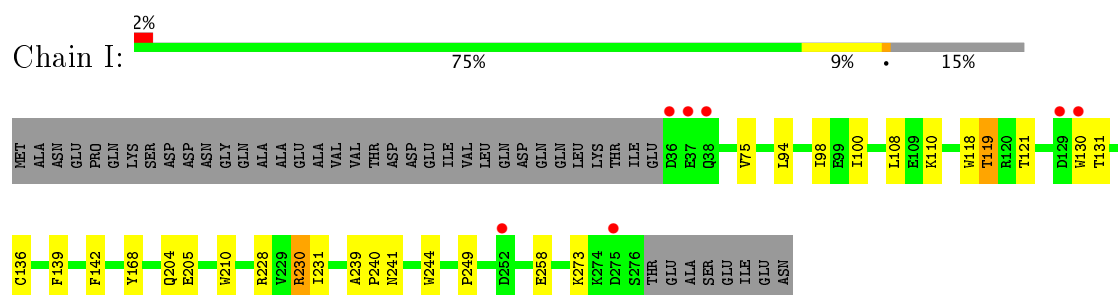
- Molecule 1: Ubiquitin thioesterase otubain-like



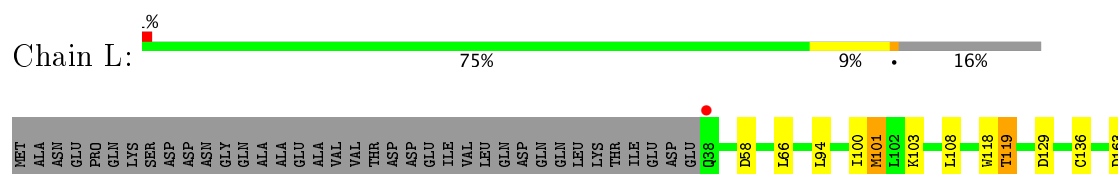
- Molecule 1: Ubiquitin thioesterase otubain-like



- Molecule 1: Ubiquitin thioesterase otubain-like

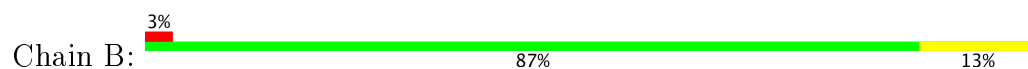


- Molecule 1: Ubiquitin thioesterase otubain-like

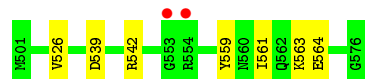




- Molecule 2: Ubiquitin aldehyde



- Molecule 2: Ubiquitin aldehyde



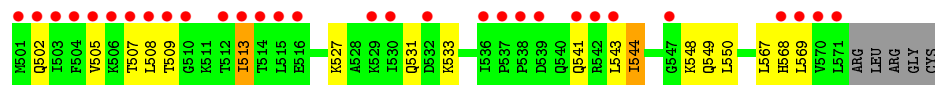
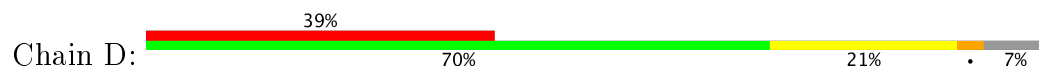
- Molecule 2: Ubiquitin aldehyde



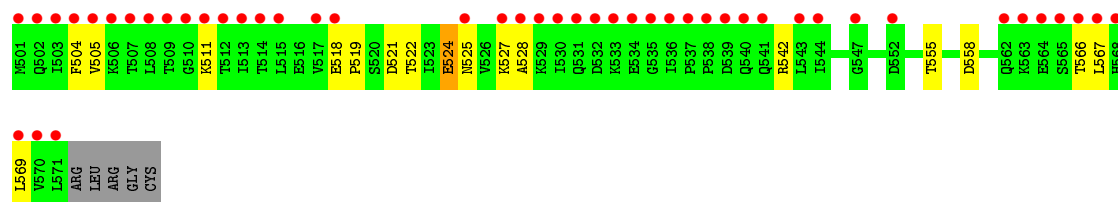
- Molecule 2: Ubiquitin aldehyde



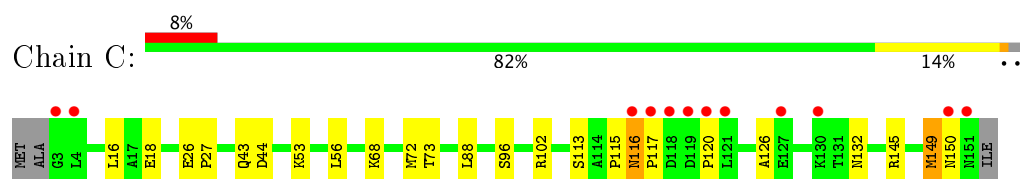
- Molecule 3: Ubiquitin



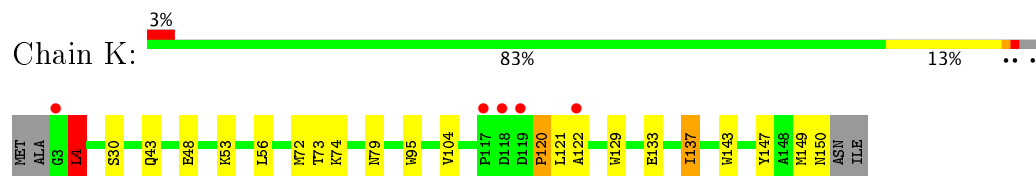
- Molecule 3: Ubiquitin



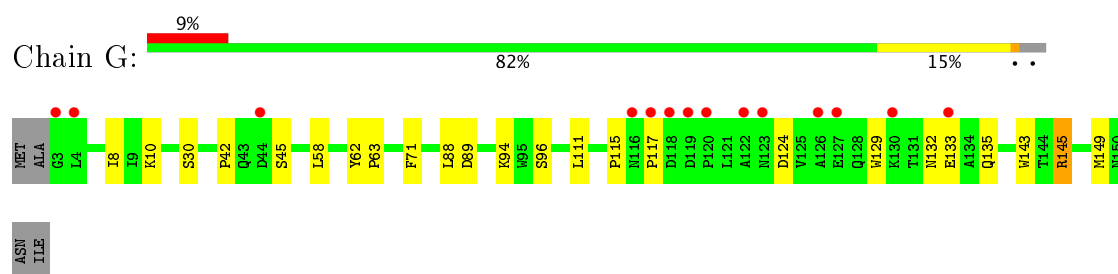
- Molecule 4: Ubiquitin-conjugating enzyme E2 N



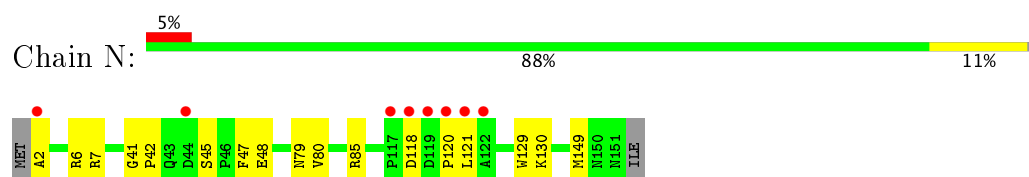
- Molecule 4: Ubiquitin-conjugating enzyme E2 N



- Molecule 4: Ubiquitin-conjugating enzyme E2 N



- Molecule 4: Ubiquitin-conjugating enzyme E2 N



4 Data and refinement statistics

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) 99.4 (39.67-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.237 0.201 , 0.234	Depositor DCC
R_{free} test set	6449 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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

All (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
1	A	244	TRP	CD2-CE2	5.60	1.48	1.41
4	G	129	TRP	CD2-CE2	5.46	1.48	1.41
1	L	118	TRP	CD2-CE2	5.29	1.47	1.41
1	E	210	TRP	CD2-CE2	5.24	1.47	1.41
1	I	118	TRP	CD2-CE2	5.16	1.47	1.41
1	L	244	TRP	CD2-CE2	5.09	1.47	1.41
1	E	244	TRP	CD2-CE2	5.03	1.47	1.41
4	G	143	TRP	CD2-CE2	5.02	1.47	1.41
4	K	95	TRP	CD2-CE2	5.01	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:E:193:ASP:OD2	2:F:542:ARG:NH2	2.21	0.73
3:H:504:PHE:O	3:H:566:THR:HA	1.90	0.71
4:K:43:GLN:HA	4:K:48:GLU:HG3	1.72	0.71
4:K:79:ASN:OD1	4:K:120:PRO:HG2	1.92	0.69
4:G:42:PRO:O	4:G:45:SER:HB3	1.93	0.69
4:C:53:LYS:HG2	4:C:73:THR:OG1	1.93	0.68
1:E:274:LYS:O	1:E:275:ASP:HB2	1.93	0.67
1:L:197:THR:CG2	1:L:200:GLN:H	2.08	0.66
4:K:53:LYS:HG2	4:K:73:THR:OG1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:541:GLN:NE2	3:D:569:LEU:HD11	2.13	0.63
3:D:541:GLN:HE21	3:D:569:LEU:HD11	1.62	0.63
1:L:101:MET:HG3	1:L:108:LEU:HB2	1.81	0.62
2:B:574:ARG:HD2	5:B:605:HOH:O	1.99	0.62
1:A:32:LYS:O	1:A:36:ASP:HB2	2.00	0.60
1:E:255:ILE:HG13	1:E:256:ALA:N	2.16	0.60
1:L:58:ASP:HA	1:L:66:LEU:HD22	1.83	0.60
1:A:214:ASP:HB3	5:A:350:HOH:O	2.03	0.58
1:I:100:ILE:HD11	1:I:258:GLU:HB3	1.86	0.57
1:I:75:VAL:HG13	1:I:273:LYS:HE3	1.85	0.57
3:D:505:VAL:O	3:D:513:ILE:HG23	2.04	0.57
1:L:163:ASP:HB3	4:N:2:ALA:HB3	1.85	0.57
4:K:4:LEU:HD12	4:K:4:LEU:H	1.70	0.56
1:I:228:ARG:HG2	1:I:249:PRO:HD2	1.88	0.55
1:I:119:THR:HG22	1:I:136:CYS:HB3	1.87	0.55
4:C:16:LEU:HD11	4:C:27:PRO:HD3	1.89	0.55
4:G:145:ARG:HA	4:G:149:MET:HG2	1.89	0.55
1:I:94:LEU:O	1:I:98:ILE:HG12	2.07	0.54
1:E:117:ASP:OD1	1:E:120:ARG:NH1	2.35	0.54
4:C:53:LYS:HE3	1:I:241:ASN:HA	1.88	0.54
1:E:97:LEU:O	1:E:101:MET:HG3	2.08	0.54
1:A:140:ILE:HD11	5:A:349:HOH:O	2.09	0.53
1:L:208:PRO:HB2	1:L:211:LYS:HG2	1.90	0.53
4:C:115:PRO:O	4:C:117:PRO:HD3	2.09	0.52
4:C:53:LYS:CE	1:I:241:ASN:HA	2.41	0.51
1:A:228:ARG:HG2	1:A:257:PRO:HA	1.93	0.51
3:D:507:THR:HG23	3:D:509:THR:H	1.74	0.51
3:H:522:THR:HA	3:H:555:THR:HA	1.93	0.51
4:K:74:LYS:HD3	4:K:147:TYR:CE2	2.46	0.51
4:N:6:ARG:HG3	4:N:7:ARG:N	2.26	0.51
4:C:120:PRO:HA	4:C:126:ALA:HB1	1.92	0.50
1:L:223:LYS:HE2	1:L:249:PRO:HB3	1.92	0.50
4:K:74:LYS:HE3	4:K:143:TRP:CZ3	2.46	0.49
4:K:53:LYS:HG3	4:K:72:MET:HB2	1.93	0.49
1:L:119:THR:HG1	1:L:136:CYS:HG	1.55	0.49
1:L:101:MET:HG2	1:L:108:LEU:HD13	1.94	0.49
1:A:228:ARG:HG3	5:A:354:HOH:O	2.12	0.48
4:K:4:LEU:CD1	4:K:4:LEU:H	2.27	0.48
1:E:255:ILE:HG13	1:E:256:ALA:H	1.79	0.47
4:K:120:PRO:O	4:K:122:ALA:N	2.48	0.47
2:J:522:THR:O	2:J:525:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:THR:HG22	1:L:200:GLN:HB2	1.97	0.46
2:B:574:ARG:NE	5:B:605:HOH:O	2.48	0.46
4:C:18:GLU:OE2	4:C:102:ARG:HD3	2.15	0.46
2:B:574:ARG:CD	5:B:605:HOH:O	2.57	0.46
3:D:544:ILE:HG13	3:D:568:HIS:HB2	1.98	0.46
1:E:250:SER:HB3	1:E:251:ASP:O	2.15	0.46
3:D:548:LYS:HE3	3:D:549:GLN:H	1.81	0.46
3:D:527:LYS:HG2	3:D:541:GLN:HG2	1.97	0.46
4:G:133:GLU:C	4:G:135:GLN:H	2.19	0.46
1:L:100:ILE:HD11	1:L:258:GLU:HB3	1.98	0.46
1:A:94:LEU:HD21	1:A:160:LEU:HD22	1.98	0.46
1:E:43:LEU:HD22	1:E:91:ARG:CZ	2.46	0.45
4:N:79:ASN:ND2	4:N:120:PRO:HD2	2.32	0.45
1:L:101:MET:CG	1:L:108:LEU:HD13	2.46	0.45
1:E:139:PHE:O	1:E:142:PHE:HB3	2.16	0.45
4:C:43:GLN:O	4:C:44:ASP:HB2	2.15	0.45
3:D:543:LEU:HD22	3:D:567:LEU:HD23	1.97	0.45
4:G:115:PRO:O	4:G:117:PRO:HD3	2.17	0.45
1:I:239:ALA:HB1	1:I:240:PRO:HD2	1.99	0.45
4:K:56:LEU:HD23	4:K:56:LEU:C	2.37	0.44
2:M:551:GLU:HG2	5:M:609:HOH:O	2.16	0.44
2:B:533:LYS:HE2	5:B:617:HOH:O	2.17	0.44
4:G:62:TYR:CD1	4:G:63:PRO:HA	2.53	0.44
3:H:505:VAL:HG23	3:H:567:LEU:HB2	1.99	0.44
4:K:149:MET:HB3	4:K:150:ASN:H	1.70	0.44
4:N:118:ASP:HB3	4:N:130:LYS:NZ	2.33	0.43
1:A:43:LEU:HD22	1:A:91:ARG:CZ	2.49	0.43
4:C:145:ARG:HA	4:C:149:MET:HG2	2.00	0.43
1:E:256:ALA:HA	1:E:257:PRO:HD2	1.88	0.43
4:G:133:GLU:O	4:G:135:GLN:N	2.42	0.43
1:A:105[A]:ARG:HD2	1:A:147:HIS:CD2	2.54	0.43
1:E:94:LEU:HD21	1:E:160:LEU:HD22	1.99	0.43
4:N:48:GLU:CD	4:N:48:GLU:H	2.21	0.43
4:C:116:ASN:HA	4:C:116:ASN:HD22	1.60	0.43
1:E:248:ILE:HG23	1:E:249:PRO:HA	2.00	0.43
4:G:132:ASN:HB3	4:G:135:GLN:HB3	2.00	0.43
4:C:56:LEU:HA	4:C:68:LYS:O	2.19	0.43
1:I:139:PHE:O	1:I:142:PHE:HB3	2.19	0.43
2:B:534:GLU:HB3	2:B:536:ILE:HG12	2.01	0.42
4:C:53:LYS:HG3	4:C:72:MET:HB2	2.00	0.42
4:G:89:ASP:HB2	4:G:94:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLY:O	3:D:548:LYS:HD3	2.19	0.42
4:C:53:LYS:CG	4:C:73:THR:OG1	2.66	0.42
3:H:525:ASN:HA	3:H:528:ALA:HB3	2.01	0.42
1:A:177:THR:HG23	1:A:220:SER:HB2	2.01	0.42
4:N:41:GLY:HA3	4:N:47:PHE:O	2.19	0.42
3:H:518:GLU:HG3	3:H:519:PRO:HD2	2.02	0.42
2:B:545:PHE:HB3	2:B:550:LEU:HD21	2.01	0.42
2:F:559:TYR:HB2	2:F:561:ILE:HD12	2.01	0.42
2:F:563:LYS:HG2	2:F:564:GLU:HG3	2.01	0.42
1:I:75:VAL:CG1	1:I:273:LYS:HE3	2.48	0.42
4:G:8:ILE:HG12	4:G:58:LEU:HD13	2.01	0.42
1:I:230:ARG:HG3	1:I:231:ILE:N	2.32	0.42
4:G:88:LEU:HD13	4:G:111:LEU:HD22	2.01	0.41
1:L:177:THR:HG23	1:L:220:SER:HB2	2.01	0.41
1:L:215:HIS:CE1	2:M:508:LEU:HD23	2.55	0.41
1:L:236:ARG:NH1	5:L:331:HOH:O	2.53	0.41
1:I:130:TRP:CZ3	1:I:131:THR:HG22	2.56	0.41
1:A:116:ARG:HA	5:A:349:HOH:O	2.20	0.41
1:E:130:TRP:HZ2	4:G:10:LYS:HB3	1.85	0.41
1:I:204:GLN:HG2	1:I:205:GLU:OE2	2.21	0.41
2:M:526:VAL:HG21	2:M:556:LEU:HD21	2.03	0.40
1:A:211:LYS:HE3	5:A:351:HOH:O	2.21	0.40
4:N:80:VAL:HA	4:N:85:ARG:O	2.21	0.40
3:H:524:GLU:HA	3:H:527:LYS:HD3	2.04	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	247/284 (87%)	236 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	243/284 (86%)	235 (97%)	6 (2%)	2 (1%)	22	24
1	I	239/284 (84%)	233 (98%)	6 (2%)	0	100	100
1	L	237/284 (84%)	230 (97%)	6 (2%)	1 (0%)	38	44
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%)	13	11
4	N	148/152 (97%)	144 (97%)	4 (3%)	0	100	100
All	All	1988/2200 (90%)	1916 (96%)	67 (3%)	5 (0%)	44	53

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 ⓘ

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%)	49	61
1	E	209/245 (85%)	201 (96%)	8 (4%)	38	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	207/245 (84%)	201 (97%)	6 (3%)	48	60
1	L	204/245 (83%)	198 (97%)	6 (3%)	48	60
2	B	67/68 (98%)	64 (96%)	3 (4%)	32	40
2	F	68/68 (100%)	66 (97%)	2 (3%)	48	60
2	J	68/68 (100%)	67 (98%)	1 (2%)	70	81
2	M	68/68 (100%)	64 (94%)	4 (6%)	23	26
3	D	65/69 (94%)	58 (89%)	7 (11%)	7	7
3	H	64/69 (93%)	59 (92%)	5 (8%)	15	16
4	C	126/129 (98%)	118 (94%)	8 (6%)	21	23
4	G	125/129 (97%)	120 (96%)	5 (4%)	36	46
4	K	124/129 (96%)	120 (97%)	4 (3%)	44	55
4	N	126/129 (98%)	124 (98%)	2 (2%)	68	79
All	All	1737/1906 (91%)	1670 (96%)	67 (4%)	37	47

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	94	LEU
1	A	124	GLU
1	A	168	TYR
1	A	252	ASP
1	A	275	ASP
2	B	509	THR
2	B	518	GLU
2	B	520	SER
1	E	36	ASP
1	E	52	ILE
1	E	61	THR
1	E	62	SER
1	E	94	LEU
1	E	168	TYR
1	E	255	ILE
1	E	270	VAL
2	F	526	VAL
2	F	539	ASP
3	D	502	GLN
3	D	508	LEU

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Mol	Chain	Res	Type
3	D	513	ILE
3	D	531	GLN
3	D	533	LYS
3	D	544	ILE
3	D	550	LEU
4	C	26	GLU
4	C	88	LEU
4	C	96	SER
4	C	113	SER
4	C	116	ASN
4	C	132	ASN
4	C	149	MET
4	C	150	ASN
1	I	108	LEU
1	I	110	LYS
1	I	119	THR
1	I	121	THR
1	I	168	TYR
1	I	230	ARG
2	J	548	LYS
4	K	4	LEU
4	K	30	SER
4	K	104	VAL
4	K	137	ILE
4	G	30	SER
4	G	71	PHE
4	G	96	SER
4	G	124	ASP
4	G	145	ARG
1	L	94	LEU
1	L	101	MET
1	L	103	LYS
1	L	119	THR
1	L	129	ASP
1	L	168	TYR
2	M	512	THR
2	M	539	ASP
2	M	562	GLN
2	M	574	ARG
3	H	511	LYS
3	H	521	ASP
3	H	524	GLU

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Mol	Chain	Res	Type
3	H	542	ARG
3	H	569	LEU
4	N	121	LEU
4	N	149	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	253	GLN
2	F	502	GLN
2	F	525	ASN
2	F	549	GLN
3	D	541	GLN
4	C	116	ASN
1	I	147	HIS
2	M	502	GLN
2	M	525	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	B	576	1,2	3,3,3	1.88	1 (33%)	1,2,2	3.01	1 (100%)
2	GLZ	F	576	1,2	3,3,3	2.27	1 (33%)	1,2,2	1.86	0
2	GLZ	J	576	1,2	3,3,3	1.99	1 (33%)	1,2,2	2.47	1 (100%)
2	GLZ	M	576	1,2	3,3,3	2.12	1 (33%)	1,2,2	2.35	1 (100%)

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	B	576	1,2	-	0/0/1/1	0/0/0/0
2	GLZ	F	576	1,2	-	0/0/1/1	0/0/0/0
2	GLZ	J	576	1,2	-	0/0/1/1	0/0/0/0
2	GLZ	M	576	1,2	-	0/0/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	576	GLZ	O-C	3.22	1.39	1.19
2	J	576	GLZ	O-C	3.38	1.40	1.19
2	M	576	GLZ	O-C	3.63	1.42	1.19
2	F	576	GLZ	O-C	3.85	1.43	1.19

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	576	GLZ	O-C-CA	-3.01	111.18	125.44
2	J	576	GLZ	O-C-CA	-2.47	113.72	125.44
2	M	576	GLZ	O-C-CA	-2.35	114.30	125.44

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	248/284 (87%)	0.25	7 (2%) 53 64	32, 45, 88, 143	0
1	E	245/284 (86%)	-0.01	7 (2%) 52 63	39, 54, 103, 137	0
1	I	241/284 (84%)	-0.03	7 (2%) 52 63	34, 51, 83, 122	0
1	L	239/284 (84%)	0.01	3 (1%) 77 85	30, 46, 80, 120	0
2	B	75/76 (98%)	0.03	2 (2%) 55 65	36, 50, 71, 77	0
2	F	75/76 (98%)	0.08	2 (2%) 55 65	44, 65, 94, 104	0
2	J	75/76 (98%)	0.05	1 (1%) 77 85	41, 58, 85, 93	0
2	M	75/76 (98%)	-0.10	0 100 100	35, 50, 67, 78	0
3	D	71/76 (93%)	1.89	30 (42%) 0 0	57, 108, 154, 159	0
3	H	71/76 (93%)	3.71	47 (66%) 0 0	102, 153, 185, 196	0
4	C	149/152 (98%)	0.35	12 (8%) 13 18	35, 49, 103, 145	0
4	G	148/152 (97%)	0.41	14 (9%) 9 14	50, 67, 111, 145	0
4	K	148/152 (97%)	0.12	5 (3%) 46 58	50, 67, 108, 142	0
4	N	150/152 (98%)	0.22	8 (5%) 27 39	36, 54, 103, 143	0
All	All	2010/2200 (91%)	0.31	145 (7%) 16 23	30, 56, 130, 196	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	514	THR	12.8
3	H	504	PHE	9.6
3	H	508	LEU	9.3
4	C	4	LEU	9.2
3	H	512	THR	8.8
3	H	501	MET	8.6
3	H	571	LEU	8.4
4	N	121	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
3	H	506	LYS	8.2
4	C	3	GLY	7.7
3	D	569	LEU	7.5
3	H	511	LYS	7.4
3	H	509	THR	7.3
3	D	512	THR	6.7
3	H	568	HIS	6.7
4	C	120	PRO	6.5
3	H	530	ILE	6.3
3	H	536	ILE	6.2
3	H	507	THR	6.1
3	H	569	LEU	6.0
3	H	505	VAL	6.0
3	H	538	PRO	6.0
3	H	502	GLN	5.7
3	H	541	GLN	5.6
4	G	122	ALA	5.6
3	H	543	LEU	5.5
3	D	509	THR	5.5
3	H	539	ASP	5.4
3	H	503	ILE	5.4
3	H	540	GLN	5.3
4	N	119	ASP	5.3
3	H	562	GLN	5.1
3	H	513	ILE	5.1
3	H	510	GLY	5.1
3	D	536	ILE	5.1
3	D	570	VAL	5.0
3	H	528	ALA	4.9
3	D	571	LEU	4.9
4	G	118	ASP	4.9
3	H	535	GLY	4.8
3	H	563	LYS	4.7
3	D	506	LYS	4.6
4	N	120	PRO	4.6
4	C	121	LEU	4.6
4	G	116	ASN	4.5
4	K	3	GLY	4.5
3	H	525	ASN	4.2
4	C	117	PRO	4.1
3	H	564	GLU	4.0
4	K	117	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
3	H	544	ILE	4.0
4	G	3	GLY	4.0
3	D	505	VAL	4.0
3	H	531	GLN	3.9
4	G	117	PRO	3.9
4	K	118	ASP	3.9
3	D	508	LEU	3.9
1	A	252	ASP	3.9
3	D	510	GLY	3.9
4	G	130	LYS	3.9
4	C	130	LYS	3.8
3	H	532	ASP	3.8
4	G	119	ASP	3.8
3	D	539	ASP	3.7
3	D	515	LEU	3.7
3	H	537	PRO	3.7
3	D	504	PHE	3.7
4	N	117	PRO	3.5
4	G	126	ALA	3.4
1	E	254	GLN	3.3
1	E	252	ASP	3.3
1	E	251	ASP	3.3
1	A	29	GLN	3.3
4	C	118	ASP	3.2
1	I	252	ASP	3.2
3	D	503	ILE	3.1
3	H	570	VAL	3.1
1	A	30	GLN	3.1
3	D	537	PRO	3.0
3	D	541	GLN	3.0
3	D	514	THR	3.0
3	D	538	PRO	2.9
3	H	517	VAL	2.9
3	D	529	LYS	2.9
3	D	513	ILE	2.9
1	L	252	ASP	2.8
3	D	507	THR	2.8
3	H	552	ASP	2.8
3	D	516	GLU	2.8
1	A	33	THR	2.8
3	H	547	GLY	2.8
4	G	123	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	H	527	LYS	2.8
4	K	119	ASP	2.8
3	H	534	GLU	2.8
3	D	542	ARG	2.7
4	K	122	ALA	2.7
4	C	127	GLU	2.7
1	E	255	ILE	2.7
3	H	533	LYS	2.7
4	C	151	ASN	2.7
3	D	530	ILE	2.6
1	E	31	LEU	2.6
3	D	532	ASP	2.6
1	A	32	LYS	2.6
3	H	567	LEU	2.6
1	I	129	ASP	2.6
4	G	120	PRO	2.5
1	I	38	GLN	2.5
3	D	543	LEU	2.5
1	I	36	ASP	2.5
2	B	575	GLY	2.5
3	H	566	THR	2.4
3	H	565	SER	2.4
4	G	4	LEU	2.4
4	N	122	ALA	2.3
1	L	253	GLN	2.3
2	F	554	ARG	2.3
4	C	150	ASN	2.3
3	H	515	LEU	2.3
4	G	133	GLU	2.3
4	N	44	ASP	2.3
3	D	547	GLY	2.3
3	H	518	GLU	2.3
3	D	502	GLN	2.3
1	E	35	GLU	2.2
4	G	127	GLU	2.2
4	G	44	ASP	2.2
1	A	209	MET	2.2
4	C	116	ASN	2.2
1	E	34	ILE	2.2
2	B	574	ARG	2.2
2	F	553	GLY	2.2
4	N	118	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	37	GLU	2.2
3	D	501	MET	2.2
1	L	38	GLN	2.1
4	N	2	ALA	2.1
1	I	130	TRP	2.1
2	J	557	SER	2.1
3	D	568	HIS	2.0
4	C	119	ASP	2.0
1	A	171	MET	2.0
1	I	275	ASP	2.0
3	H	529	LYS	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLZ	F	576	4/4	0.91	0.25	-	61,64,67,71	0
2	GLZ	M	576	4/4	0.96	0.11	-	44,47,50,52	0
2	GLZ	B	576	4/4	0.96	0.30	-	50,54,57,63	0
2	GLZ	J	576	4/4	0.98	0.11	-	50,53,54,54	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.