



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:23 am BST

PDB ID : 3TMP  
Title : The catalytic domain of human deubiquitinase DUBA in complex with ubiquitin aldehyde  
Authors : Ma, X.; Yin, J.; Hymowitz, S.; Starovasnik, M.; Cochran, A.  
Deposited on : 2011-08-31  
Resolution : 1.91 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

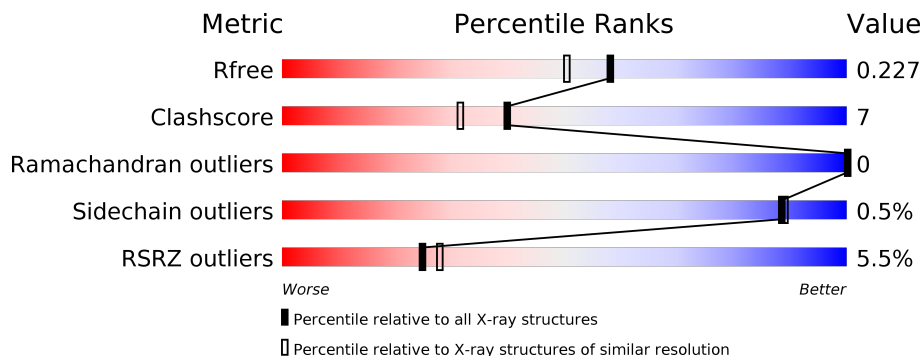
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	184	
1	C	184	
1	E	184	
1	G	184	
2	B	76	
2	D	76	

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Mol	Chain	Length	Quality of chain
2	F	76	 80% 18%
2	H	76	 89% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLZ	B	76	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8666 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 OTU domain-containing protein 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	166	1369	849	242	267	1	10	0	0	0
1	C	168	1377	855	242	267	1	12	0	0	0
1	E	169	1380	855	243	269	1	12	0	0	0
1	G	154	1290	803	227	249	1	10	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLY	-	EXPRESSION TAG	UNP Q96G74
A	169	SER	-	EXPRESSION TAG	UNP Q96G74
A	170	HIS	-	EXPRESSION TAG	UNP Q96G74
A	171	MET	-	EXPRESSION TAG	UNP Q96G74
C	168	GLY	-	EXPRESSION TAG	UNP Q96G74
C	169	SER	-	EXPRESSION TAG	UNP Q96G74
C	170	HIS	-	EXPRESSION TAG	UNP Q96G74
C	171	MET	-	EXPRESSION TAG	UNP Q96G74
E	168	GLY	-	EXPRESSION TAG	UNP Q96G74
E	169	SER	-	EXPRESSION TAG	UNP Q96G74
E	170	HIS	-	EXPRESSION TAG	UNP Q96G74
E	171	MET	-	EXPRESSION TAG	UNP Q96G74
G	168	GLY	-	EXPRESSION TAG	UNP Q96G74
G	169	SER	-	EXPRESSION TAG	UNP Q96G74
G	170	HIS	-	EXPRESSION TAG	UNP Q96G74
G	171	MET	-	EXPRESSION TAG	UNP Q96G74

- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	D	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	F	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
2	H	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

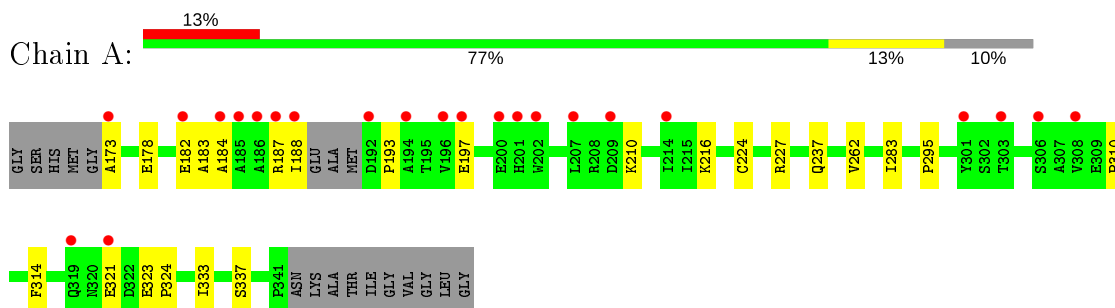
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total	O	0	0
			147	147		
3	B	63	Total	O	0	0
			63	63		
3	C	151	Total	O	0	0
			151	151		
3	D	50	Total	O	0	0
			50	50		
3	E	169	Total	O	0	0
			169	169		
3	F	59	Total	O	0	0
			59	59		
3	G	139	Total	O	0	0
			139	139		
3	H	68	Total	O	0	0
			68	68		

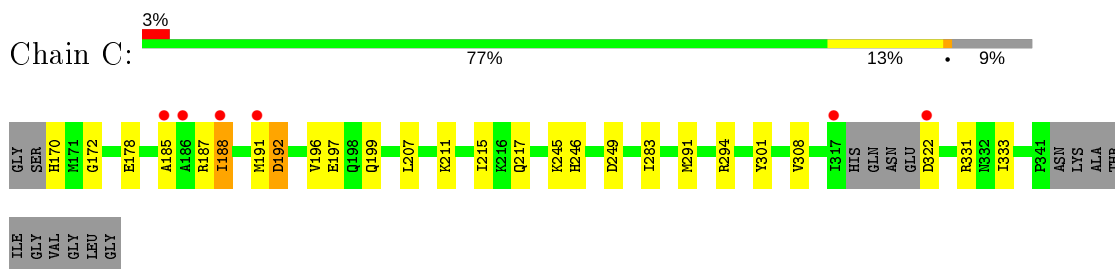
### 3 Residue-property plots [i](#)

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.

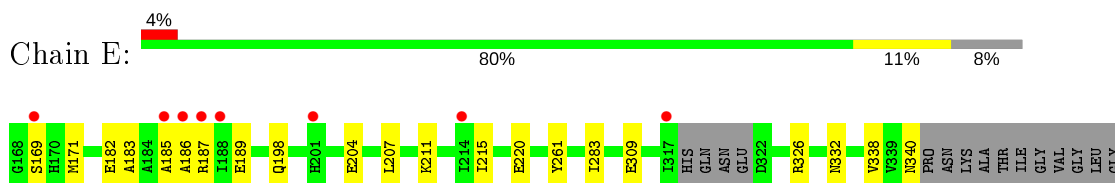
- Molecule 1: OTU domain-containing protein 5



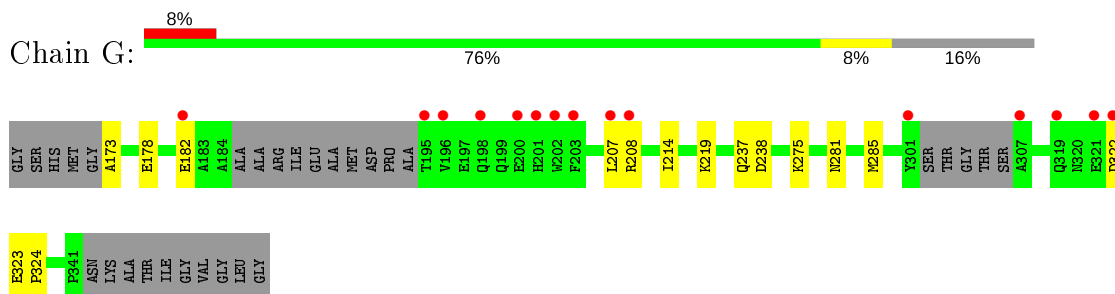
- Molecule 1: OTU domain-containing protein 5




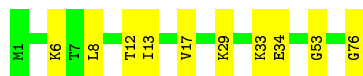
- Molecule 1: OTU domain-containing protein 5



- Molecule 1: OTU domain-containing protein 5




## ● Molecule 2: Polyubiquitin-C

Chain B:  87% 13%


## ● Molecule 2: Polyubiquitin-C

Chain D:  92% 8%

## ● Molecule 2: Polyubiquitin-C

Chain F:  80% 18%

## ● Molecule 2: Polyubiquitin-C

Chain H:  89% 11%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.53Å 65.30Å 65.84Å 90.26° 93.53° 99.28°	Depositor
Resolution (Å)	46.35 – 1.91 46.35 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.35-1.91) 97.6 (46.35-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.32	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.190 , 0.227 0.190 , 0.227	Depositor DCC
$R_{free}$ test set	3749 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtrriage
Anisotropy	0.239	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8499e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.47	0/1390	0.54	0/1875
1	C	0.58	0/1398	0.60	0/1884
1	E	0.55	0/1400	0.56	0/1885
1	G	0.54	0/1309	0.58	0/1762
2	B	0.44	0/603	0.56	0/811
2	D	0.48	0/603	0.60	0/811
2	F	0.46	0/603	0.61	0/811
2	H	0.49	0/603	0.60	0/811
All	All	0.52	0/7909	0.58	0/10650

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
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	75	GLY	Mainchain

## 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	1369	0	1264	21	0
1	C	1377	0	1275	23	0
1	E	1380	0	1276	31	0
1	G	1290	0	1185	9	0
2	B	601	0	629	11	0
2	D	601	0	628	4	0
2	F	601	0	628	15	0
2	H	601	0	628	7	0
3	A	147	0	0	3	0
3	B	63	0	0	3	0
3	C	151	0	0	5	0
3	D	50	0	0	1	2
3	E	169	0	0	4	2
3	F	59	0	0	2	0
3	G	139	0	0	3	2
3	H	68	0	0	3	0
All	All	8666	0	7513	112	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 7.

All (112) 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:A:224:CYS:SG	2:B:76:GLZ:C	2.16	1.31
1:E:186:ALA:HA	1:E:189:GLU:OE1	1.52	1.07
2:D:49:GLN:NE2	3:D:778:HOH:O	1.88	1.06
1:C:170:HIS:N	3:C:158:HOH:O	1.89	1.04
1:E:171:MET:CE	1:E:182:GLU:HG3	1.97	0.94
1:A:224:CYS:SG	2:B:76:GLZ:HXT	2.06	0.94
1:A:173:ALA:HA	1:A:178:GLU:OE2	1.71	0.90
1:E:171:MET:HE1	1:E:182:GLU:HG3	1.53	0.88
1:E:169:SER:OG	1:E:171:MET:HG3	1.76	0.84
1:C:187:ARG:O	1:C:191:MET:HG2	1.77	0.83
1:E:169:SER:OG	1:E:171:MET:CE	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238:ASP:OD1	3:G:687:HOH:O	1.99	0.80
1:A:224:CYS:HG	2:B:76:GLZ:C	1.91	0.80
1:A:323:GLU:HG3	1:A:324:PRO:HD2	1.65	0.79
1:C:294:ARG:HG2	1:C:322:ASP:HB3	1.64	0.78
1:A:187:ARG:O	1:A:188:ILE:HB	1.85	0.76
2:F:24:GLU:OE2	3:F:736:HOH:O	2.04	0.75
2:F:63:LYS:HE2	2:F:64:GLU:OE2	1.88	0.73
1:E:169:SER:OG	1:E:171:MET:HE3	1.87	0.72
2:F:54:ARG:HH11	2:F:54:ARG:HG3	1.53	0.72
1:A:321:GLU:OE2	3:A:799:HOH:O	2.07	0.71
1:E:171:MET:CE	1:E:182:GLU:CG	2.69	0.70
1:E:185:ALA:O	1:E:189:GLU:HG3	1.91	0.70
1:G:275:LYS:NZ	3:G:692:HOH:O	2.10	0.70
2:H:34:GLU:OE2	3:H:506:HOH:O	2.11	0.69
1:G:281:ASN:O	1:G:285:MET:HG3	1.94	0.68
1:C:197:GLU:OE1	3:C:483:HOH:O	2.12	0.68
1:C:185:ALA:O	1:C:188:ILE:N	2.27	0.67
2:B:13:ILE:HD11	2:B:34:GLU:HG3	1.75	0.67
1:A:224:CYS:SG	2:B:76:GLZ:CA	2.85	0.65
2:B:17:VAL:HG12	2:B:29:LYS:HE3	1.81	0.62
2:D:5:VAL:HG21	2:D:30:ILE:HD11	1.81	0.62
1:E:183:ALA:O	1:E:187:ARG:HG3	1.99	0.61
1:C:191:MET:HE3	1:C:196:VAL:HG22	1.84	0.60
1:C:188:ILE:HD13	1:C:191:MET:HG3	1.84	0.59
1:E:198:GLN:NE2	3:E:791:HOH:O	2.35	0.58
1:E:171:MET:HE3	1:E:182:GLU:HB2	1.84	0.58
2:F:54:ARG:HG3	2:F:54:ARG:NH1	2.18	0.58
1:A:262:VAL:HG22	1:A:283:ILE:HD13	1.85	0.57
1:E:169:SER:OG	1:E:171:MET:HE2	2.05	0.56
1:C:211:LYS:HD2	1:C:308:VAL:HG23	1.87	0.56
1:G:173:ALA:HB3	1:G:178:GLU:OE1	2.06	0.55
1:C:331:ARG:HH21	1:C:333:ILE:HD11	1.72	0.55
1:A:310:PRO:O	3:A:371:HOH:O	2.17	0.55
1:C:283:ILE:HD13	2:D:8:LEU:HD11	1.88	0.55
1:C:246:HIS:HB3	1:C:291:MET:SD	2.48	0.54
1:E:171:MET:HE3	1:E:182:GLU:CB	2.37	0.54
1:E:198:GLN:NE2	3:E:808:HOH:O	2.39	0.54
1:C:187:ARG:O	1:C:191:MET:CG	2.53	0.53
1:E:204:GLU:HG2	1:E:215:ILE:HD12	1.89	0.53
2:F:24:GLU:CG	2:F:52:ASP:HB3	2.38	0.53
1:A:187:ARG:O	1:A:188:ILE:CB	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:CD1	1:C:215:ILE:HD11	2.40	0.52
2:H:63:LYS:HG2	2:H:64:GLU:HG3	1.90	0.51
1:E:171:MET:HE3	1:E:182:GLU:CG	2.40	0.51
1:E:283:ILE:HD13	2:F:8:LEU:HD21	1.93	0.50
1:A:193:PRO:O	1:A:197:GLU:HB2	2.11	0.50
1:E:185:ALA:O	1:E:189:GLU:CG	2.59	0.49
1:C:245:LYS:HE2	1:C:249:ASP:OD2	2.12	0.49
1:E:171:MET:HE1	1:E:182:GLU:CG	2.33	0.49
2:B:8:LEU:O	3:B:779:HOH:O	2.20	0.49
1:E:340:ASN:HB3	3:E:551:HOH:O	2.13	0.49
2:H:54:ARG:NE	2:H:58:ASP:OD2	2.44	0.49
1:A:210:LYS:O	3:A:531:HOH:O	2.20	0.49
1:C:188:ILE:CD1	1:C:191:MET:HG3	2.42	0.49
2:F:40:GLN:HG3	2:F:40:GLN:O	2.12	0.49
1:E:326:ARG:HB3	1:E:338:VAL:HB	1.95	0.48
2:B:53:GLY:O	3:B:232:HOH:O	2.20	0.48
1:C:191:MET:CE	1:C:196:VAL:HG22	2.42	0.48
1:C:192:ASP:OD1	1:C:192:ASP:N	2.34	0.48
2:H:69:LEU:C	2:H:69:LEU:HD23	2.34	0.48
1:E:220:GLU:OE1	3:E:715:HOH:O	2.20	0.48
1:C:199:GLN:HG2	1:C:301:TYR:CE2	2.49	0.48
1:A:188:ILE:HD11	1:A:333:ILE:HG21	1.96	0.47
1:C:172:GLY:O	1:C:178:GLU:HB2	2.15	0.47
2:H:40:GLN:NE2	3:H:813:HOH:O	2.33	0.47
1:A:182:GLU:HG2	1:A:183:ALA:N	2.30	0.47
1:C:217:GLN:HG3	3:C:109:HOH:O	2.15	0.47
1:E:211:LYS:NZ	1:E:309:GLU:OE2	2.43	0.47
1:E:171:MET:CE	1:E:182:GLU:CB	2.92	0.46
2:B:6:LYS:HD3	2:B:12:THR:OG1	2.16	0.46
1:E:187:ARG:NE	1:E:332:ASN:OD1	2.48	0.46
2:F:63:LYS:CE	2:F:64:GLU:OE2	2.61	0.46
2:F:16:GLU:HB2	3:F:393:HOH:O	2.15	0.45
1:E:171:MET:HE1	1:E:182:GLU:HA	1.97	0.45
1:A:227:ARG:HB3	1:A:237:GLN:HB2	1.99	0.45
1:C:170:HIS:ND1	3:C:722:HOH:O	2.22	0.44
1:E:169:SER:CB	1:E:171:MET:HG3	2.46	0.44
2:F:24:GLU:HG3	2:F:52:ASP:HB3	1.99	0.44
2:B:33:LYS:NZ	1:G:182:GLU:OE2	2.47	0.44
1:A:216:LYS:HB3	1:A:337:SER:HB3	1.99	0.44
2:F:23:ILE:HG22	2:F:27:LYS:HE3	1.99	0.44
1:C:187:ARG:NH1	1:C:191:MET:HE1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:TYR:CG	2:F:8:LEU:HD13	2.53	0.43
1:G:219:LYS:HG3	1:G:237:GLN:OE1	2.17	0.43
1:G:323:GLU:HG2	1:G:324:PRO:HD2	2.00	0.43
2:D:22:THR:OG1	2:D:25:ASN:HB2	2.18	0.43
2:B:8:LEU:HD12	3:B:779:HOH:O	2.18	0.43
1:A:182:GLU:HG2	1:A:183:ALA:H	1.83	0.42
1:A:184:ALA:O	1:A:188:ILE:HD12	2.20	0.42
1:E:207:LEU:HA	1:E:207:LEU:HD23	1.89	0.42
2:F:37:PRO:HA	2:F:38:PRO:HD3	1.93	0.42
1:G:208:ARG:HG2	1:G:214:ILE:CD1	2.49	0.42
2:H:63:LYS:HG3	3:H:254:HOH:O	2.19	0.42
1:E:185:ALA:O	1:E:189:GLU:CD	2.58	0.41
3:G:728:HOH:O	2:H:74:ARG:HD3	2.20	0.41
1:E:261:TYR:CD2	2:F:8:LEU:HD13	2.55	0.41
1:A:262:VAL:HG22	1:A:283:ILE:CD1	2.49	0.41
1:G:207:LEU:HA	1:G:207:LEU:HD23	1.87	0.41
1:C:331:ARG:HD3	3:C:482:HOH:O	2.20	0.41
1:A:295:PRO:HA	1:A:314:PHE:O	2.21	0.40
2:F:48:LYS:HE2	2:F:59:TYR:HE1	1.87	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)
3:D:770:HOH:O	3:G:777:HOH:O[1_545]	1.75	0.45
3:E:715:HOH:O	3:G:684:HOH:O[1_546]	2.03	0.17
3:D:615:HOH:O	3:E:372:HOH:O[1_554]	2.17	0.03

## 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	161/184 (88%)	156 (97%)	5 (3%)	0	100	100
1	C	163/184 (89%)	161 (99%)	2 (1%)	0	100	100
1	E	164/184 (89%)	157 (96%)	7 (4%)	0	100	100
1	G	147/184 (80%)	142 (97%)	5 (3%)	0	100	100
2	B	74/76 (97%)	74 (100%)	0	0	100	100
2	D	74/76 (97%)	74 (100%)	0	0	100	100
2	F	74/76 (97%)	74 (100%)	0	0	100	100
2	H	74/76 (97%)	74 (100%)	0	0	100	100
All	All	931/1040 (90%)	912 (98%)	19 (2%)	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	144/155 (93%)	144 (100%)	0	100	100
1	C	144/155 (93%)	142 (99%)	2 (1%)	67	63
1	E	144/155 (93%)	144 (100%)	0	100	100
1	G	136/155 (88%)	135 (99%)	1 (1%)	84	83
2	B	68/68 (100%)	68 (100%)	0	100	100
2	D	68/68 (100%)	68 (100%)	0	100	100
2	F	68/68 (100%)	67 (98%)	1 (2%)	65	61
2	H	68/68 (100%)	68 (100%)	0	100	100
All	All	840/892 (94%)	836 (100%)	4 (0%)	88	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	188	ILE
1	C	192	ASP

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Mol	Chain	Res	Type
2	F	8	LEU
1	G	322	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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
1	SEP	E	177	1	8,9,10	1.46	1 (12%)	8,12,14	1.58	1 (12%)
2	GLZ	H	76	2	3,3,3	0.72	0	0,2,2	0.00	-
2	GLZ	B	76	2	3,3,3	0.55	0	0,2,2	0.00	-
2	GLZ	F	76	2	3,3,3	0.44	0	0,2,2	0.00	-
1	SEP	G	177	1	8,9,10	1.44	1 (12%)	8,12,14	1.38	2 (25%)
2	GLZ	D	76	2	3,3,3	0.82	0	0,2,2	0.00	-
1	SEP	A	177	1	8,9,10	1.29	1 (12%)	8,12,14	1.52	3 (37%)
1	SEP	C	177	1	8,9,10	1.34	1 (12%)	8,12,14	1.38	1 (12%)

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
1	SEP	E	177	1	-	1/5/8/10	-
2	GLZ	H	76	2	-	0/0/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLZ	B	76	2	-	0/0/1/1	-
2	GLZ	F	76	2	-	0/0/1/1	-
1	SEP	G	177	1	-	1/5/8/10	-
2	GLZ	D	76	2	-	0/0/1/1	-
1	SEP	A	177	1	-	1/5/8/10	-
1	SEP	C	177	1	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	177	SEP	P-O1P	3.10	1.60	1.50
1	C	177	SEP	P-O1P	2.90	1.59	1.50
1	G	177	SEP	P-O1P	2.78	1.59	1.50
1	A	177	SEP	P-O1P	2.60	1.58	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	SEP	OG-CB-CA	3.81	111.86	108.14
1	A	177	SEP	OG-CB-CA	2.87	110.94	108.14
1	C	177	SEP	OG-CB-CA	2.86	110.92	108.14
1	G	177	SEP	OG-CB-CA	2.39	110.47	108.14
1	G	177	SEP	O2P-P-OG	2.15	112.46	106.73
1	A	177	SEP	O3P-P-OG	2.11	112.36	106.73
1	A	177	SEP	O2P-P-OG	2.01	112.07	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	177	SEP	CA-CB-OG-P
1	G	177	SEP	CA-CB-OG-P
1	A	177	SEP	CA-CB-OG-P
1	C	177	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	76	GLZ	4	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	165/184 (89%)	0.75	23 (13%) 2 3	14, 26, 51, 67	0
1	C	167/184 (90%)	0.29	6 (3%) 42 46	11, 21, 38, 49	0
1	E	168/184 (91%)	0.42	8 (4%) 30 34	11, 24, 39, 52	0
1	G	153/184 (83%)	0.52	15 (9%) 7 9	8, 23, 52, 63	0
2	B	75/76 (98%)	0.14	0 100 100	14, 27, 38, 43	0
2	D	75/76 (98%)	0.20	0 100 100	11, 27, 40, 44	0
2	F	75/76 (98%)	0.18	0 100 100	12, 27, 38, 42	0
2	H	75/76 (98%)	0.16	0 100 100	14, 25, 37, 39	0
All	All	953/1040 (91%)	0.39	52 (5%) 25 28	8, 25, 46, 67	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	185	ALA	9.2
1	G	301	TYR	7.1
1	E	317	ILE	5.5
1	A	202	TRP	5.4
1	E	186	ALA	5.3
1	A	321	GLU	4.9
1	G	196	VAL	4.6
1	A	188	ILE	4.5
1	G	202	TRP	4.2
1	A	185	ALA	4.2
1	A	196	VAL	4.1
1	C	191	MET	4.1
1	G	203	PHE	4.1
1	A	306	SER	4.1
1	A	182	GLU	4.0
1	G	321	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	322	ASP	3.7
1	A	186	ALA	3.4
1	G	307	ALA	3.3
1	A	194	ALA	3.3
1	A	301	TYR	3.2
1	G	200	GLU	3.2
1	G	198	GLN	3.1
1	E	188	ILE	3.1
1	A	319	GLN	3.0
1	C	186	ALA	3.0
1	G	182	GLU	3.0
1	G	208	ARG	2.8
1	A	187	ARG	2.8
1	G	322	ASP	2.8
1	A	201	HIS	2.8
1	A	192	ASP	2.8
1	C	317	ILE	2.7
1	A	200	GLU	2.7
1	G	201	HIS	2.7
1	A	308	VAL	2.7
1	A	214	ILE	2.6
1	A	303	THR	2.6
1	C	185	ALA	2.6
1	E	187	ARG	2.6
1	G	207	LEU	2.6
1	A	184	ALA	2.5
1	E	201	HIS	2.5
1	E	169	SER	2.4
1	G	319	GLN	2.4
1	A	173	ALA	2.4
1	A	207	LEU	2.3
1	G	195	THR	2.3
1	A	209	ASP	2.3
1	A	197	GLU	2.3
1	E	214	ILE	2.2
1	C	188	ILE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	GLZ	F	76	4/4	0.85	0.16	13,17,18,20	0
2	GLZ	B	76	4/4	0.87	0.16	26,26,27,27	0
2	GLZ	H	76	4/4	0.91	0.09	19,20,22,22	0
2	GLZ	D	76	4/4	0.95	0.10	13,14,14,16	0
1	SEP	A	177	10/11	0.97	0.11	16,20,22,24	0
1	SEP	E	177	10/11	0.98	0.10	11,14,15,16	0
1	SEP	G	177	10/11	0.98	0.09	14,17,21,22	0
1	SEP	C	177	10/11	0.98	0.10	9,11,13,14	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.