



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:00 PM GMT

PDB ID : 4QMK  
Title : Crystal structure of type III effector protein ExoU (exoU)  
Authors : Halavaty, A.S.; Tyson, G.H.; Zhang, A.; Hauser, A.R.; Anderson, W.F.; Center  
for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2014-06-16  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

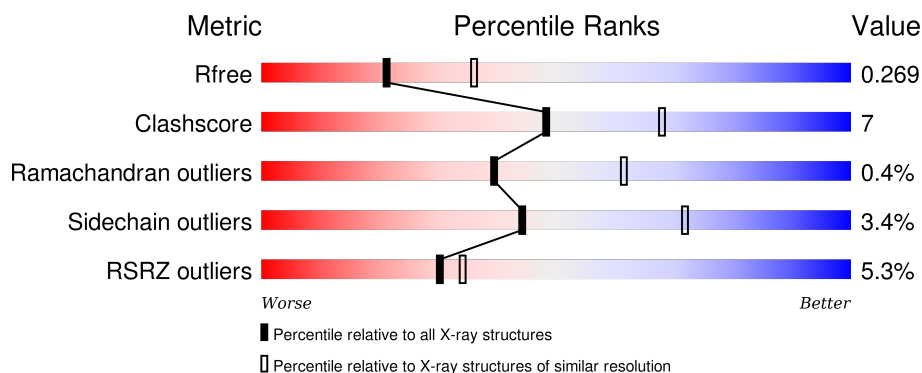
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	677	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>13%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	677	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>10%</div> <div>•</div> <div>25%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8162 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 Type III secretion system effector protein ExoU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	3	0
			4056	2542	741	762	11			
1	B	509	Total	C	N	O	S	0	2	0
			3895	2438	708	738	11			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP I2BZ03
A	-10	GLY	-	EXPRESSION TAG	UNP I2BZ03
A	-9	LYS	-	EXPRESSION TAG	UNP I2BZ03
A	-8	ALA	-	EXPRESSION TAG	UNP I2BZ03
A	-7	SER	-	EXPRESSION TAG	UNP I2BZ03
A	-6	VAL	-	EXPRESSION TAG	UNP I2BZ03
A	-5	ASP	-	EXPRESSION TAG	UNP I2BZ03
A	-4	GLN	-	EXPRESSION TAG	UNP I2BZ03
A	-3	ILE	-	EXPRESSION TAG	UNP I2BZ03
A	-2	SER	-	EXPRESSION TAG	UNP I2BZ03
A	-1	LYS	-	EXPRESSION TAG	UNP I2BZ03
A	0	LEU	-	EXPRESSION TAG	UNP I2BZ03
A	640	GLY	-	EXPRESSION TAG	UNP I2BZ03
A	641	GLY	-	EXPRESSION TAG	UNP I2BZ03
A	642	ARG	-	EXPRESSION TAG	UNP I2BZ03
A	643	LEU	-	EXPRESSION TAG	UNP I2BZ03
A	644	VAL	-	EXPRESSION TAG	UNP I2BZ03
A	645	PRO	-	EXPRESSION TAG	UNP I2BZ03
A	646	ARG	-	EXPRESSION TAG	UNP I2BZ03
A	647	GLY	-	EXPRESSION TAG	UNP I2BZ03
A	648	SER	-	EXPRESSION TAG	UNP I2BZ03
A	649	PRO	-	EXPRESSION TAG	UNP I2BZ03
A	650	GLY	-	EXPRESSION TAG	UNP I2BZ03
A	651	ALA	-	EXPRESSION TAG	UNP I2BZ03
A	652	ALA	-	EXPRESSION TAG	UNP I2BZ03

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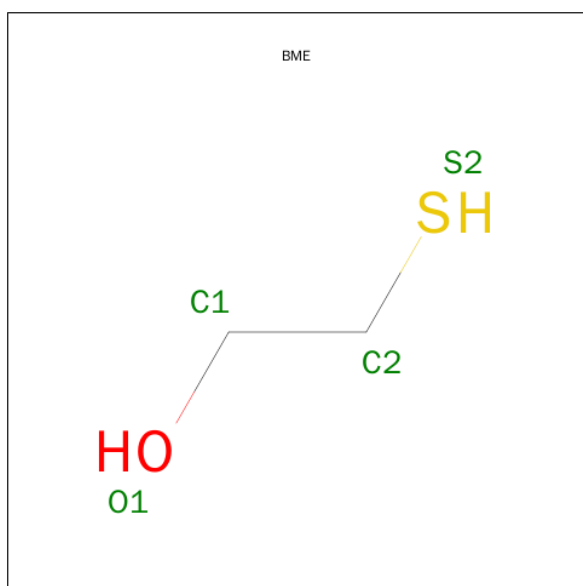
Chain	Residue	Modelled	Actual	Comment	Reference
A	653	GLY	-	EXPRESSION TAG	UNP I2BZ03
A	654	HIS	-	EXPRESSION TAG	UNP I2BZ03
A	655	ASN	-	EXPRESSION TAG	UNP I2BZ03
A	656	HIS	-	EXPRESSION TAG	UNP I2BZ03
A	657	ASN	-	EXPRESSION TAG	UNP I2BZ03
A	658	HIS	-	EXPRESSION TAG	UNP I2BZ03
A	659	ASN	-	EXPRESSION TAG	UNP I2BZ03
A	660	HIS	-	EXPRESSION TAG	UNP I2BZ03
A	661	ASN	-	EXPRESSION TAG	UNP I2BZ03
A	662	HIS	-	EXPRESSION TAG	UNP I2BZ03
A	663	ASN	-	EXPRESSION TAG	UNP I2BZ03
A	664	HIS	-	EXPRESSION TAG	UNP I2BZ03
A	665	ASN	-	EXPRESSION TAG	UNP I2BZ03
B	-11	MET	-	EXPRESSION TAG	UNP I2BZ03
B	-10	GLY	-	EXPRESSION TAG	UNP I2BZ03
B	-9	LYS	-	EXPRESSION TAG	UNP I2BZ03
B	-8	ALA	-	EXPRESSION TAG	UNP I2BZ03
B	-7	SER	-	EXPRESSION TAG	UNP I2BZ03
B	-6	VAL	-	EXPRESSION TAG	UNP I2BZ03
B	-5	ASP	-	EXPRESSION TAG	UNP I2BZ03
B	-4	GLN	-	EXPRESSION TAG	UNP I2BZ03
B	-3	ILE	-	EXPRESSION TAG	UNP I2BZ03
B	-2	SER	-	EXPRESSION TAG	UNP I2BZ03
B	-1	LYS	-	EXPRESSION TAG	UNP I2BZ03
B	0	LEU	-	EXPRESSION TAG	UNP I2BZ03
B	640	GLY	-	EXPRESSION TAG	UNP I2BZ03
B	641	GLY	-	EXPRESSION TAG	UNP I2BZ03
B	642	ARG	-	EXPRESSION TAG	UNP I2BZ03
B	643	LEU	-	EXPRESSION TAG	UNP I2BZ03
B	644	VAL	-	EXPRESSION TAG	UNP I2BZ03
B	645	PRO	-	EXPRESSION TAG	UNP I2BZ03
B	646	ARG	-	EXPRESSION TAG	UNP I2BZ03
B	647	GLY	-	EXPRESSION TAG	UNP I2BZ03
B	648	SER	-	EXPRESSION TAG	UNP I2BZ03
B	649	PRO	-	EXPRESSION TAG	UNP I2BZ03
B	650	GLY	-	EXPRESSION TAG	UNP I2BZ03
B	651	ALA	-	EXPRESSION TAG	UNP I2BZ03
B	652	ALA	-	EXPRESSION TAG	UNP I2BZ03
B	653	GLY	-	EXPRESSION TAG	UNP I2BZ03
B	654	HIS	-	EXPRESSION TAG	UNP I2BZ03
B	655	ASN	-	EXPRESSION TAG	UNP I2BZ03
B	656	HIS	-	EXPRESSION TAG	UNP I2BZ03

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Chain	Residue	Modelled	Actual	Comment	Reference
B	657	ASN	-	EXPRESSION TAG	UNP I2BZ03
B	658	HIS	-	EXPRESSION TAG	UNP I2BZ03
B	659	ASN	-	EXPRESSION TAG	UNP I2BZ03
B	660	HIS	-	EXPRESSION TAG	UNP I2BZ03
B	661	ASN	-	EXPRESSION TAG	UNP I2BZ03
B	662	HIS	-	EXPRESSION TAG	UNP I2BZ03
B	663	ASN	-	EXPRESSION TAG	UNP I2BZ03
B	664	HIS	-	EXPRESSION TAG	UNP I2BZ03
B	665	ASN	-	EXPRESSION TAG	UNP I2BZ03

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).

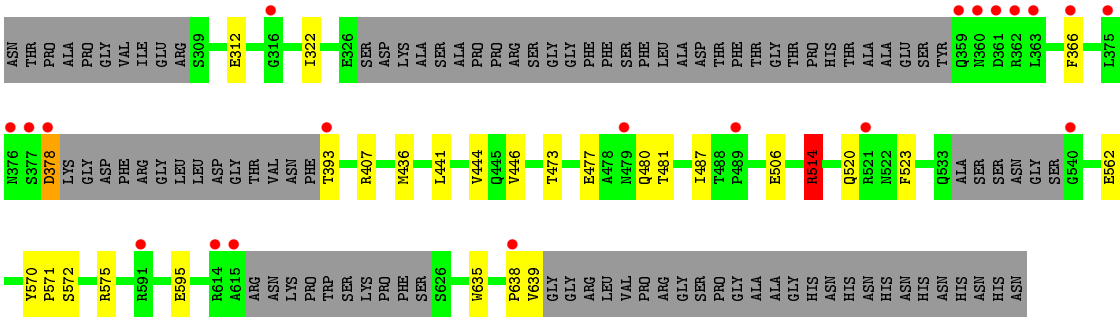


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	1
			137	137		
3	B	70	Total	O	0	0
			70	70		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.22Å 115.34Å 88.44Å 90.00° 102.77° 90.00°	Depositor
Resolution (Å)	29.86 – 2.50 29.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.86-2.50) 94.9 (29.86-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.206 , 0.270 0.208 , 0.269	Depositor DCC
$R_{free}$ test set	2190 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43205 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: BME

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	0.77	0/4120	0.85	4/5576 (0.1%)
1	B	0.62	0/3950	0.80	2/5346 (0.0%)
All	All	0.70	0/8070	0.82	6/10922 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	A	106	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	514	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	A	245	LEU	CA-CB-CG	5.57	128.12	115.30
1	A	504	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	423	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4056	0	4132	62	0
1	B	3895	0	3963	59	0
2	A	4	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	137	0	0	5	0
3	B	70	0	0	7	0
All	All	8162	0	8100	117	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 7.

All (117) 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:B:251:ASN:HB3	3:B:722:HOH:O	1.53	1.05
1:A:160:THR:HG21	1:B:160:THR:HG21	1.56	0.87
1:B:67:ILE:O	1:B:70:PRO:HD2	1.78	0.83
1:A:64:ALA:HB1	1:A:385:LEU:HD22	1.60	0.82
1:B:570[A]:TYR:HB3	1:B:571:PRO:HD3	1.69	0.75
1:A:622:LYS:HB3	1:A:623:PRO:CD	2.18	0.74
1:A:203:ILE:HD12	1:A:217:ASP:OD1	1.90	0.70
1:B:78:GLU:OE1	1:B:407:ARG:NH2	2.24	0.70
1:A:78:GLU:OE1	1:A:407:ARG:NH2	2.21	0.69
1:B:203:ILE:HD12	1:B:217:ASP:OD1	1.94	0.68
1:A:144:VAL:CG2	1:A:157:LEU:HD12	2.26	0.66
1:B:520:GLN:HG3	1:B:523:PHE:HB2	1.78	0.66
1:A:520:GLN:HG3	1:A:523:PHE:HB2	1.78	0.65
1:B:64:ALA:HB1	3:B:739:HOH:O	1.96	0.65
1:A:506:GLU:HG3	3:A:816:HOH:O	1.98	0.64
1:A:570:TYR:HB3	1:A:571:PRO:HD3	1.78	0.63
1:B:144:VAL:CG2	1:B:157:LEU:HD12	2.29	0.63
1:B:436:MET:CE	1:B:441:LEU:HD13	2.29	0.62
1:B:35:LEU:HD23	1:B:444:VAL:HG11	1.81	0.61
1:B:268:LEU:N	1:B:269:PRO:HD2	2.15	0.61
1:B:35:LEU:HD23	1:B:444:VAL:CG1	2.31	0.61
1:A:436:MET:CE	1:A:441:LEU:HD13	2.31	0.61
1:A:35:LEU:HD23	1:A:444:VAL:HG11	1.82	0.60
1:B:170:GLN:HB3	1:B:171:PRO:HD2	1.84	0.60
1:A:622:LYS:HB3	1:A:623:PRO:HD2	1.84	0.59
1:A:173:GLU:HG2	1:A:177:ARG:HH22	1.67	0.59
1:A:35:LEU:HD23	1:A:444:VAL:CG1	2.33	0.58
1:A:622:LYS:CB	1:A:623:PRO:CD	2.82	0.57
1:A:206:ARG:NH2	1:A:217:ASP:OD2	2.38	0.57
1:B:206:ARG:NH2	1:B:217:ASP:OD2	2.38	0.57
1:A:520:GLN:HG2	1:A:523:PHE:CD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD12	3:B:758:HOH:O	2.05	0.56
1:B:78:GLU:OE1	1:B:407:ARG:CZ	2.55	0.55
1:A:130:THR:HG23	1:A:267:ALA:HB1	1.89	0.55
1:A:242:ARG:HG2	1:A:575:ARG:HG3	1.88	0.54
1:A:64:ALA:O	1:A:67:ILE:HG22	2.08	0.54
1:B:322:ILE:HD13	1:B:366:PHE:CE1	2.42	0.54
1:B:520:GLN:HG2	1:B:523:PHE:CD2	2.44	0.53
1:B:119:LEU:N	1:B:120:PRO:HD2	2.24	0.52
1:A:260:ARG:O	1:A:264:ILE:HG12	2.09	0.52
1:B:473:THR:O	1:B:477:GLU:HG2	2.09	0.52
1:B:242:ARG:HG2	1:B:575:ARG:HG3	1.92	0.52
1:A:164:ARG:HH11	1:A:164:ARG:HB3	1.74	0.52
1:B:150:PRO:HB3	1:B:635:TRP:CE2	2.45	0.52
1:A:161:LEU:HD11	1:B:143:LEU:HD21	1.92	0.52
1:A:520:GLN:CG	1:A:523:PHE:CD2	2.92	0.52
1:B:234:THR:HG22	1:B:235:GLY:N	2.24	0.51
1:A:473:THR:O	1:A:477:GLU:HG2	2.11	0.51
1:A:461:ARG:HB3	3:A:915:HOH:O	2.11	0.51
1:B:105:MET:HE2	1:B:110:PHE:HA	1.93	0.51
1:B:260:ARG:O	1:B:264:ILE:HG12	2.11	0.51
1:A:384:GLY:C	1:A:386:LEU:H	2.14	0.51
1:A:520:GLN:HG3	1:A:523:PHE:CG	2.47	0.50
1:B:63:GLY:HA2	1:B:119:LEU:HD11	1.93	0.49
1:A:105:MET:HE2	1:A:110:PHE:HA	1.94	0.49
1:A:638:PRO:O	1:A:639:VAL:HB	2.12	0.49
1:B:638:PRO:O	1:B:639:VAL:HB	2.13	0.49
1:A:234:THR:HG22	1:A:235:GLY:N	2.28	0.48
1:A:119:LEU:N	1:A:120:PRO:HD2	2.27	0.48
1:A:164:ARG:HE	1:A:177:ARG:NH2	2.12	0.48
1:A:146:SER:HB2	1:A:624:PHE:CD1	2.48	0.48
1:A:146:SER:HB2	1:A:624:PHE:CE1	2.49	0.48
1:B:520:GLN:CG	1:B:523:PHE:CD2	2.97	0.47
1:B:102:ALA:HA	1:B:229:LYS:HB2	1.97	0.47
1:B:436:MET:CE	1:B:441:LEU:CD1	2.93	0.46
1:A:245:LEU:HD22	1:A:570:TYR:CE2	2.50	0.46
1:A:65:LYS:HD2	1:A:325:PHE:CD1	2.50	0.46
1:A:520:GLN:HG3	1:A:523:PHE:CB	2.43	0.46
1:A:553:GLN:HB3	3:A:847:HOH:O	2.15	0.46
1:B:520:GLN:HG3	1:B:523:PHE:CB	2.45	0.46
1:B:184:ILE:HG23	1:B:221:LEU:HD21	1.99	0.45
1:A:62:GLY:HA3	1:A:65:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LYS:HB3	3:B:755:HOH:O	2.16	0.45
1:A:151:VAL:HG22	3:A:831:HOH:O	2.15	0.45
1:B:150:PRO:HB3	1:B:635:TRP:NE1	2.31	0.45
1:B:138:SER:HB3	3:B:747:HOH:O	2.17	0.45
1:A:35:LEU:CD2	1:A:444:VAL:HG11	2.46	0.45
1:A:39:ARG:HH22	1:A:451:ASP:CG	2.21	0.44
1:B:378:ASP:OD1	1:B:378:ASP:N	2.41	0.44
1:A:626:SER:OG	1:A:626:SER:O	2.25	0.44
1:B:322:ILE:HD13	1:B:366:PHE:CD1	2.53	0.44
1:A:118:ASP:OD1	1:A:121:ARG:HG2	2.18	0.44
1:B:570[A]:TYR:CB	1:B:571:PRO:HD3	2.45	0.44
1:B:520:GLN:HG3	1:B:523:PHE:CG	2.53	0.44
1:A:102:ALA:HA	1:A:229:LYS:HB2	1.99	0.44
1:B:312:GLU:OE2	1:B:514:ARG:NH1	2.51	0.44
1:A:436:MET:CE	1:A:441:LEU:CD1	2.95	0.43
1:B:446:VAL:HG13	3:B:710:HOH:O	2.18	0.43
1:A:181:ARG:HD3	1:A:207:LEU:O	2.18	0.43
1:A:322:ILE:HD13	1:A:366:PHE:CE2	2.52	0.43
1:B:480:GLN:HA	3:B:718:HOH:O	2.18	0.43
1:B:119:LEU:N	1:B:120:PRO:CD	2.82	0.43
1:A:312:GLU:H	1:A:312:GLU:HG3	1.66	0.42
1:B:234:THR:CG2	1:B:235:GLY:N	2.82	0.42
1:A:161:LEU:HD21	1:B:157:LEU:HD21	2.02	0.42
1:B:506:GLU:H	1:B:506:GLU:CD	2.23	0.42
1:B:188:ILE:O	1:B:196:ARG:NH2	2.53	0.42
1:A:143:LEU:CD1	1:B:143:LEU:HD22	2.50	0.42
1:B:35:LEU:CD2	1:B:444:VAL:HG11	2.47	0.42
1:A:127:ASP:HA	1:A:128:PRO:HD3	1.94	0.42
1:B:35:LEU:HD11	1:B:47:VAL:HG13	2.01	0.42
1:A:379:LYS:HB2	1:A:401:HIS:NE2	2.34	0.42
1:A:64:ALA:HB1	1:A:385:LEU:CD2	2.42	0.42
1:A:205:GLU:HG3	3:A:907:HOH:O	2.20	0.41
1:A:145:ARG:NH1	1:A:244:GLN:OE1	2.50	0.41
1:A:629:VAL:HG12	1:A:633:LYS:HE3	2.03	0.41
1:A:119:LEU:N	1:A:120:PRO:CD	2.83	0.41
1:B:487:ILE:O	1:B:487:ILE:HG13	2.21	0.41
1:A:173:GLU:HG2	1:A:177:ARG:NH2	2.35	0.41
1:B:181:ARG:HD3	1:B:207:LEU:O	2.20	0.41
1:B:119:LEU:HA	1:B:122:LEU:HB2	2.02	0.41
1:B:312:GLU:CD	1:B:514:ARG:HH12	2.25	0.41
1:B:181:ARG:NH1	1:B:210:GLY:HA2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PHE:N	1:A:70:PRO:CD	2.84	0.41
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.88	0.40
1:B:105:MET:CE	1:B:110:PHE:HA	2.51	0.40
1:B:113:LEU:C	1:B:113:LEU:HD23	2.42	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	517/677 (76%)	497 (96%)	16 (3%)	4 (1%)	24	41
1	B	493/677 (73%)	477 (97%)	16 (3%)	0	100	100
All	All	1010/1354 (75%)	974 (96%)	32 (3%)	4 (0%)	39	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ALA
1	A	385	LEU
1	A	622	LYS
1	A	196	ARG

### 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	433/548 (79%)	419 (97%)	14 (3%)	46	74
1	B	416/548 (76%)	401 (96%)	15 (4%)	42	69
All	All	849/1096 (78%)	820 (97%)	29 (3%)	44	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	78	GLU
1	A	164	ARG
1	A	175	LEU
1	A	244	GLN
1	A	245	LEU
1	A	312	GLU
1	A	392	PHE
1	A	394	MET
1	A	481	THR
1	A	489	PRO
1	A	562	GLU
1	A	572	SER
1	A	595	GLU
1	B	78	GLU
1	B	122	LEU
1	B	139	GLU
1	B	177	ARG
1	B	196	ARG
1	B	199	GLU
1	B	244	GLN
1	B	268	LEU
1	B	378	ASP
1	B	393	THR
1	B	481	THR
1	B	514	ARG
1	B	562	GLU
1	B	572	SER
1	B	595	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	BME	A	700	1	3,3,3	0.62	0	2,2,2	0.05	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	BME	A	700	1	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	528/677 (77%)	-0.11	15 (2%) 56 61	20, 43, 85, 133	0
1	B	509/677 (75%)	0.29	40 (7%) 15 17	29, 63, 106, 151	0
All	All	1037/1354 (76%)	0.09	55 (5%) 30 34	20, 52, 101, 151	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	GLY	6.9
1	B	540	GLY	6.8
1	B	393	THR	5.5
1	B	615	ALA	5.4
1	B	359	GLN	4.7
1	A	362	ARG	4.3
1	A	392	PHE	4.1
1	A	121	ARG	3.7
1	A	308	ARG	3.6
1	B	224	HIS	3.6
1	B	200	VAL	3.6
1	B	212	GLY	3.6
1	B	211	GLY	3.4
1	B	591	ARG	3.3
1	B	210	GLY	3.3
1	B	614	ARG	3.3
1	B	209	ALA	3.2
1	B	360	ASN	3.2
1	B	361	ASP	3.1
1	B	198	PRO	3.1
1	B	489	PRO	3.0
1	A	361	ASP	3.0
1	B	479	ASN	3.0
1	B	521	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	375	LEU	2.9
1	B	197	PRO	2.8
1	B	199	GLU	2.8
1	B	203	ILE	2.8
1	A	393	THR	2.7
1	A	378	ASP	2.7
1	B	638	PRO	2.7
1	A	622	LYS	2.7
1	B	108	LYS	2.7
1	B	362	ARG	2.6
1	B	378	ASP	2.5
1	B	222	SER	2.5
1	B	377	SER	2.5
1	B	97	CYS	2.5
1	A	626	SER	2.4
1	B	41	SER	2.4
1	B	220	VAL	2.4
1	B	363	LEU	2.4
1	B	202	ALA	2.4
1	B	376	ASN	2.3
1	B	366	PHE	2.3
1	A	195	ASN	2.3
1	B	190	GLY	2.3
1	B	316	GLY	2.2
1	B	124	ASN	2.2
1	A	194	ALA	2.1
1	A	120	PRO	2.0
1	B	207	LEU	2.0
1	B	189	ALA	2.0
1	A	364	GLN	2.0
1	A	366	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BME	A	700	4/4	0.89	0.19	0.39	77,80,81,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.