



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 02:42 PM EDT

PDB ID : 3DEC  
Title : Crystal structure of a glycosyl hydrolases family 2 protein from Bacteroides thetaiotaomicron  
Authors : Kumaran, D.; Bonanno, J.; Romero, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-06-09  
Resolution : 2.80 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.

---

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	:	2.23.2
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)	:	2.23.2

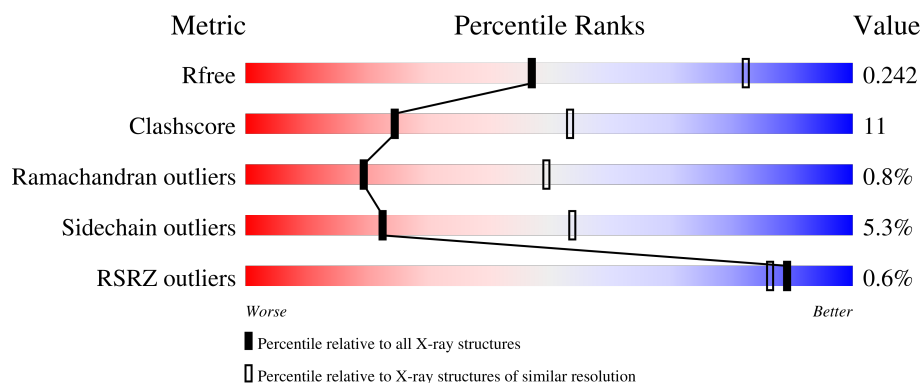
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	1000	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8048 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	983	Total	C	N	O	S	Se	0	2	0
			7949	5066	1356	1498	15	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q8A2X6
A	2	LEU	-	expression tag	UNP Q8A2X6
A	512	VAL	ALA	engineered mutation	UNP Q8A2X6
A	999	GLU	-	expression tag	UNP Q8A2X6
A	1000	GLY	-	expression tag	UNP Q8A2X6

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total	O	0	0
			98	98		

### 3 Residue-property plots

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: Beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.06Å 211.07Å 71.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-2.80) 95.5 (19.98-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.68 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.184 , 0.243 0.185 , 0.242	Depositor DCC
$R_{free}$ test set	1491 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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, 0.333 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: K

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	0.67	0/8153	0.75	2/11051 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LEU	CA-CB-CG	8.06	133.84	115.30
1	A	498	CYS	CA-CB-SG	-6.27	102.71	114.00

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	7949	0	7690	171	0
2	A	1	0	0	0	0
3	A	98	0	0	1	0
All	All	8048	0	7690	171	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 11.

All (171) 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:256:THR:HG22	1:A:317:ALA:CB	1.76	1.16
1:A:621:ILE:HD12	1:A:629:ARG:HB2	1.20	1.10
1:A:106:MSE:HE1	1:A:581:PRO:HG2	1.35	1.07
1:A:621:ILE:HD11	1:A:629:ARG:CZ	1.86	1.06
1:A:234:GLU:HG3	1:A:236:GLU:OE1	1.64	0.97
1:A:256:THR:HG22	1:A:317:ALA:HB2	1.47	0.95
1:A:621:ILE:CD1	1:A:629:ARG:HB2	1.98	0.94
1:A:159:GLU:HB2	1:A:178:LYS:HD3	1.53	0.90
1:A:98:GLU:HG2	1:A:416:HIS:CE1	2.07	0.89
1:A:37:THR:HG22	1:A:37:THR:O	1.74	0.85
1:A:328:LYS:HE2	1:A:402[B]:ARG:HH12	1.42	0.83
1:A:256:THR:HG22	1:A:317:ALA:HB1	1.62	0.82
1:A:37:THR:O	1:A:37:THR:CG2	2.27	0.81
1:A:611:LYS:O	1:A:614:GLN:HG2	1.80	0.81
1:A:106:MSE:CE	1:A:581:PRO:HG2	2.10	0.80
1:A:621:ILE:HD12	1:A:629:ARG:CB	2.08	0.79
1:A:457:LEU:HD22	1:A:470:THR:HG22	1.65	0.78
1:A:459:ASN:ND2	1:A:460:GLU:HG3	2.01	0.76
1:A:522:LEU:HD23	1:A:525:TYR:CB	2.17	0.74
1:A:722:TRP:C	1:A:724:GLY:H	1.91	0.74
1:A:287:ILE:N	1:A:287:ILE:HD13	2.03	0.72
1:A:722:TRP:O	1:A:724:GLY:N	2.22	0.72
1:A:834:GLN:HG3	1:A:991:THR:HG22	1.73	0.71
1:A:100:TYR:CE1	1:A:417:GLY:HA3	2.26	0.71
1:A:531:ASN:OD1	1:A:877:ARG:NH1	2.23	0.71
1:A:175:ILE:HD12	1:A:179:LEU:HD21	1.72	0.70
1:A:834:GLN:HG3	1:A:991:THR:CG2	2.22	0.70
1:A:643:ILE:HD11	1:A:696:LYS:HG3	1.74	0.69
1:A:857:ASN:ND2	1:A:859:THR:OG1	2.27	0.68
1:A:457:LEU:HD22	1:A:470:THR:CG2	2.23	0.67
1:A:866:LEU:HG	1:A:910:ARG:HG2	1.79	0.65
1:A:234:GLU:OE1	1:A:240:GLU:HB3	1.98	0.63
1:A:159:GLU:CB	1:A:178:LYS:HD3	2.27	0.62
1:A:129:THR:HG22	1:A:185:THR:HG22	1.81	0.62
1:A:328:LYS:HE2	1:A:402[B]:ARG:NH1	2.13	0.61
1:A:814:LYS:HG2	1:A:843:TRP:CZ2	2.35	0.61
1:A:540:TRP:O	1:A:544:GLU:HG3	1.99	0.61
1:A:722:TRP:C	1:A:724:GLY:N	2.50	0.61
1:A:33:VAL:HG11	1:A:326:GLY:HA3	1.83	0.61
1:A:94:ILE:HD12	1:A:192:ARG:HH22	1.66	0.61
1:A:459:ASN:ND2	1:A:460:GLU:CG	2.64	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD22	1:A:292:GLN:HE21	1.66	0.61
1:A:602:PRO:HB3	1:A:606:LEU:HD23	1.83	0.60
1:A:522:LEU:HD23	1:A:525:TYR:HB2	1.83	0.60
1:A:234:GLU:CG	1:A:236:GLU:OE1	2.46	0.60
1:A:45:MSE:HE2	1:A:216:LEU:HD22	1.83	0.60
1:A:849:ARG:NH1	1:A:962:ASP:OD2	2.35	0.60
1:A:231:SER:HB2	1:A:331:PHE:CD1	2.36	0.60
1:A:670:THR:HG22	1:A:671:VAL:N	2.17	0.59
1:A:256:THR:CG2	1:A:317:ALA:CB	2.68	0.59
1:A:893:MSE:HE1	1:A:934:ALA:HB3	1.84	0.59
1:A:264:LYS:HE3	1:A:268:ASP:OD1	2.03	0.59
1:A:453:VAL:HG23	1:A:454:ILE:HG12	1.84	0.59
1:A:621:ILE:CD1	1:A:629:ARG:CZ	2.72	0.59
1:A:498:CYS:O	1:A:499:ARG:C	2.40	0.59
1:A:58:ASN:ND2	1:A:119:LYS:HG2	2.19	0.58
1:A:349:LEU:HD13	1:A:540:TRP:HZ3	1.68	0.58
1:A:522:LEU:HD23	1:A:525:TYR:HB3	1.84	0.58
1:A:94:ILE:HD12	1:A:192:ARG:NH2	2.19	0.57
1:A:663:VAL:HG21	1:A:673:LEU:HD22	1.88	0.56
1:A:389:HIS:HA	1:A:410:GLU:OE1	2.05	0.56
1:A:621:ILE:HD11	1:A:629:ARG:NH2	2.21	0.56
1:A:256:THR:CG2	1:A:317:ALA:HB1	2.34	0.55
1:A:896:TYR:HB3	1:A:948:ILE:HD13	1.87	0.55
1:A:621:ILE:CD1	1:A:629:ARG:NH2	2.69	0.55
1:A:33:VAL:CG1	1:A:326:GLY:HA3	2.36	0.55
1:A:512:VAL:O	1:A:512:VAL:HG13	2.08	0.54
1:A:161:LEU:HD21	1:A:178:LYS:HD2	1.88	0.54
1:A:168:LYS:HE3	1:A:363:ARG:HD3	1.90	0.54
1:A:621:ILE:HD11	1:A:629:ARG:NE	2.23	0.53
1:A:893:MSE:HE3	1:A:934:ALA:O	2.08	0.53
1:A:643:ILE:HD11	1:A:696:LYS:CG	2.38	0.53
1:A:95:TYR:CE1	1:A:591:CYS:HB3	2.44	0.53
1:A:332:ARG:HD3	1:A:332:ARG:C	2.29	0.52
1:A:440:ARG:O	1:A:444:GLU:HG2	2.08	0.52
1:A:808:ILE:HG22	1:A:816:VAL:HB	1.92	0.52
1:A:622:ASP:OD1	1:A:625:ASN:ND2	2.43	0.52
1:A:667:PRO:O	1:A:668:HIS:HB2	2.10	0.51
1:A:867:GLY:O	1:A:883:ILE:HA	2.11	0.51
1:A:57:LYS:O	1:A:58:ASN:CB	2.58	0.51
1:A:7:TRP:HB3	1:A:151:PHE:CG	2.46	0.50
1:A:28:ALA:HB2	1:A:42:PRO:CD	2.42	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLN:HG2	1:A:389:HIS:HB2	1.94	0.50
1:A:622:ASP:HB3	1:A:627:THR:HB	1.91	0.50
1:A:118:TYR:CD2	1:A:118:TYR:C	2.85	0.50
1:A:498:CYS:O	1:A:499:ARG:O	2.30	0.50
1:A:461:ALA:HB1	3:A:1171:HOH:O	2.10	0.50
1:A:767:THR:HA	1:A:901:GLN:HB2	1.94	0.50
1:A:421:GLY:O	1:A:427:LYS:NZ	2.45	0.49
1:A:256:THR:HG22	1:A:317:ALA:CA	2.38	0.49
1:A:384:THR:HB	1:A:406:TYR:HB2	1.93	0.49
1:A:106:MSE:CE	1:A:581:PRO:CG	2.87	0.49
1:A:98:GLU:CG	1:A:416:HIS:CE1	2.89	0.49
1:A:57:LYS:O	1:A:58:ASN:HB3	2.12	0.49
1:A:735:GLU:HB2	1:A:745:SER:HB3	1.95	0.49
1:A:819:ALA:HA	1:A:836:THR:O	2.14	0.48
1:A:772:ARG:HD2	1:A:972:THR:HA	1.95	0.48
1:A:191:TYR:N	1:A:191:TYR:CD2	2.80	0.48
1:A:116:VAL:HB	1:A:117:PRO:CD	2.44	0.48
1:A:812:THR:O	1:A:812:THR:CG2	2.62	0.48
1:A:94:ILE:HG21	1:A:101:GLU:HB2	1.96	0.48
1:A:53:PHE:HB2	1:A:79:ILE:HG22	1.95	0.47
1:A:403:TYR:CG	1:A:701:LEU:HD11	2.49	0.47
1:A:7:TRP:HB3	1:A:151:PHE:CD2	2.50	0.47
1:A:249:VAL:O	1:A:285:ASN:HB2	2.14	0.47
1:A:408:ILE:HG23	1:A:454:ILE:HB	1.95	0.47
1:A:617:LYS:HG3	1:A:633:TRP:HD1	1.79	0.47
1:A:584:VAL:O	1:A:585:PRO:C	2.52	0.47
1:A:511:VAL:O	1:A:511:VAL:HG22	2.14	0.47
1:A:680:LEU:HB3	1:A:684:ILE:HD11	1.97	0.47
1:A:762:LEU:HD12	1:A:788:LEU:HD11	1.97	0.47
1:A:256:THR:O	1:A:317:ALA:HB2	2.15	0.46
1:A:161:LEU:CD2	1:A:178:LYS:HD2	2.45	0.46
1:A:351:LYS:HG2	1:A:540:TRP:CH2	2.49	0.46
1:A:485:TYR:CE2	1:A:487:ARG:HB2	2.51	0.46
1:A:174:ASP:C	1:A:174:ASP:OD1	2.52	0.46
1:A:670:THR:CG2	1:A:671:VAL:N	2.78	0.46
1:A:52:LYS:HE3	1:A:52:LYS:HA	1.97	0.45
1:A:812:THR:O	1:A:812:THR:HG22	2.17	0.45
1:A:53:PHE:HB2	1:A:79:ILE:CG2	2.47	0.45
1:A:723:ASN:H	1:A:723:ASN:HD22	1.63	0.45
1:A:532:SER:H	1:A:605:HIS:HD2	1.65	0.45
1:A:779:LEU:HD23	1:A:846:SER:HB2	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLN:NE2	1:A:523:CYS:SG	2.90	0.44
1:A:332:ARG:C	1:A:332:ARG:CD	2.86	0.44
1:A:387:ASN:O	1:A:389:HIS:N	2.51	0.44
1:A:45:MSE:CE	1:A:216:LEU:HD22	2.48	0.44
1:A:149:ILE:HG23	1:A:208:SER:HA	1.99	0.44
1:A:465:ILE:HG13	1:A:469:ARG:HE	1.82	0.44
1:A:316:ASP:HB2	1:A:320:LYS:H	1.83	0.43
1:A:622:ASP:CG	1:A:625:ASN:ND2	2.71	0.43
1:A:814:LYS:HE2	1:A:843:TRP:CE2	2.53	0.43
1:A:934:ALA:HA	1:A:958:THR:O	2.18	0.43
1:A:316:ASP:HB3	1:A:318:GLY:H	1.83	0.43
1:A:643:ILE:CD1	1:A:696:LYS:HG3	2.47	0.43
1:A:116:VAL:HB	1:A:117:PRO:HD2	2.00	0.43
1:A:663:VAL:HG11	1:A:671:VAL:HG11	2.00	0.42
1:A:459:ASN:HD22	1:A:460:GLU:HG3	1.80	0.42
1:A:609:VAL:O	1:A:613:TYR:HB2	2.19	0.42
1:A:621:ILE:HD13	1:A:629:ARG:NH2	2.34	0.42
1:A:234:GLU:O	1:A:234:GLU:HG2	2.18	0.42
1:A:337:LYS:O	1:A:338:ASN:C	2.57	0.42
1:A:365:VAL:CG1	1:A:370:MSE:HG3	2.50	0.42
1:A:484:GLN:NE2	1:A:498:CYS:SG	2.92	0.42
1:A:622:ASP:OD2	1:A:624:LYS:HG2	2.20	0.42
1:A:644:LEU:HD11	1:A:691:LEU:HD22	2.02	0.42
1:A:775:MSE:HE1	1:A:845:LYS:O	2.20	0.42
1:A:328:LYS:CE	1:A:402[B]:ARG:HH12	2.22	0.42
1:A:463:ASN:OD1	1:A:464:GLY:N	2.52	0.42
1:A:631:LYS:HE2	1:A:633:TRP:CE2	2.53	0.42
1:A:119:LYS:HE2	1:A:119:LYS:HB2	1.74	0.42
1:A:432:LEU:HB3	1:A:433:PRO:HD3	2.02	0.41
1:A:102:PHE:HB2	1:A:117:PRO:HG2	2.03	0.41
1:A:167:SER:OG	1:A:200:GLU:OE1	2.34	0.41
1:A:475:LYS:NZ	1:A:495:ASP:OD2	2.52	0.41
1:A:21:HIS:ND1	1:A:22:THR:O	2.32	0.41
1:A:265:ASP:C	1:A:265:ASP:OD1	2.59	0.41
1:A:355:ARG:HD2	1:A:377:MSE:HE1	2.01	0.41
1:A:432:LEU:N	1:A:433:PRO:CD	2.84	0.41
1:A:784:GLY:HA2	1:A:786:HIS:CE1	2.56	0.41
1:A:432:LEU:HD22	1:A:469:ARG:NH1	2.36	0.41
1:A:365:VAL:HG12	1:A:370:MSE:HG3	2.01	0.41
1:A:501:TYR:CZ	1:A:524:GLU:HB3	2.55	0.41
1:A:584:VAL:O	1:A:584:VAL:HG13	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:GLU:O	1:A:612:ILE:HG12	2.20	0.41
1:A:725:LYS:HE2	1:A:995:TYR:OH	2.21	0.40
1:A:935:LEU:HA	1:A:936:PRO:HD3	1.86	0.40
1:A:457:LEU:CD2	1:A:470:THR:HG22	2.44	0.40
1:A:161:LEU:HD23	1:A:178:LYS:HE2	2.03	0.40
1:A:297:VAL:HG22	1:A:298:ARG:N	2.36	0.40
1:A:332:ARG:NH2	1:A:452:VAL:O	2.55	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	977/1000 (98%)	918 (94%)	51 (5%)	8 (1%)	<b>19</b> 49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	SER
1	A	499	ARG
1	A	58	ASN
1	A	447	LYS
1	A	723	ASN
1	A	841	THR
1	A	268	ASP
1	A	493	ASN

### 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	856/853 (100%)	811 (95%)	45 (5%)	22	54

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	35	LYS
1	A	37	THR
1	A	159	GLU
1	A	188	LEU
1	A	208	SER
1	A	222	GLN
1	A	234	GLU
1	A	256	THR
1	A	269	LYS
1	A	275	SER
1	A	286	LEU
1	A	287	ILE
1	A	291	GLU
1	A	332	ARG
1	A	363	ARG
1	A	384	THR
1	A	415	SER
1	A	469	ARG
1	A	474	LEU
1	A	498	CYS
1	A	512	VAL
1	A	520	PHE
1	A	523	CYS
1	A	567	LYS
1	A	590	PHE
1	A	621	ILE
1	A	625	ASN
1	A	679	GLN
1	A	682	LYS
1	A	683	THR
1	A	684	ILE
1	A	772	ARG
1	A	779	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	797	GLU
1	A	799	LYS
1	A	805	GLN
1	A	849	ARG
1	A	918	SER
1	A	920	LYS
1	A	928	SER
1	A	941	LEU
1	A	952	GLU
1	A	991	THR
1	A	997	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	GLN
1	A	416	HIS
1	A	459	ASN
1	A	484	GLN
1	A	605	HIS
1	A	660	ASN
1	A	723	ASN
1	A	857	ASN
1	A	879	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	969/1000 (96%)	-0.58	6 (0%) 89 86	14, 30, 48, 59	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	LYS	3.1
1	A	729	ALA	2.9
1	A	462	GLY	2.7
1	A	515	ASP	2.5
1	A	422	PRO	2.4
1	A	181	ASP	2.3

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	Q<0.9
2	K	A	1101	1/1	0.99	0.05	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.