



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:27 am BST

PDB ID : 2C9K  
Title : Structure of the functional form of the mosquito-larvicidal Cry4Aa toxin from *Bacillus thuringiensis* at 2.8 Å resolution  
Authors : Boonserm, P.; Mo, M.; Angsuthanasombat, C.; Lescar, J.  
Deposited on : 2005-12-13  
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 : 2.11  
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

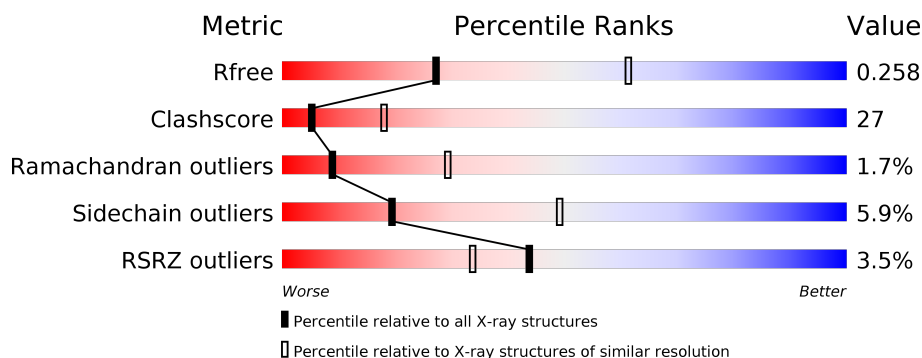
# 1 Overall quality at a glance

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 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	612	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>38%</div> <div>5% •</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5057 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.

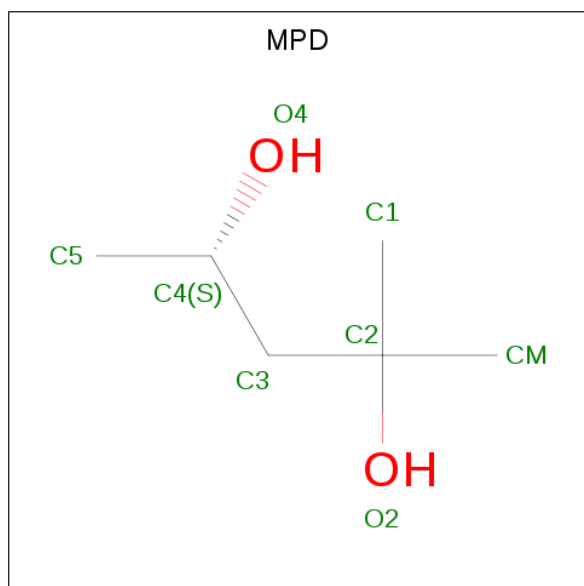
- Molecule 1 is a protein called PESTICIDAL CRYSTAL PROTEIN CRY4AA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	598	4811	3097	788	918	8	27	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	GLU	ASN	conflict	UNP P16480

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	8	6	2	0	0

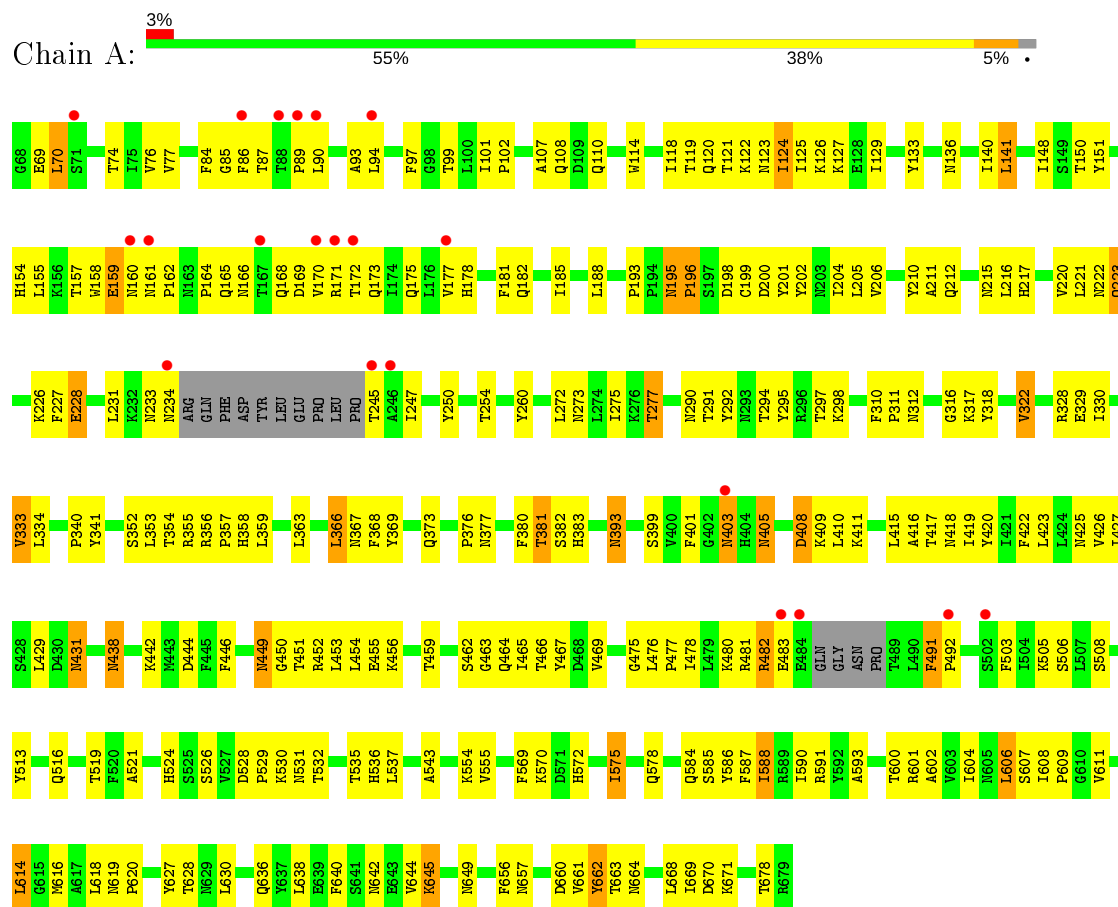
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	238	Total 238	O 238	0	0

### 3 Residue-property plots

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: PESTICIDAL CRYSTAL PROTEIN CRY4AA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.20 Å   202.07 Å   98.73 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	7.00 – 2.80 83.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (7.00-2.80) 100.0 (83.13-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.82 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.203   ,   0.259 0.210   ,   0.258	Depositor DCC
$R_{free}$ test set	1172 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: MPD

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	0.37	0/4933	0.61	1/6728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	587	PHE	N-CA-C	-5.15	97.11	111.00

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	4811	0	4682	252	1
2	A	8	0	14	4	0
3	A	238	0	0	38	0
All	All	5057	0	4696	252	1

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 27.

All (252) 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:158:TRP:HE1	1:A:168:GLN:HG2	1.11	1.10
1:A:645:LYS:H	1:A:645:LYS:HE2	1.16	1.06
1:A:223:GLN:HE22	1:A:227:PHE:HB2	1.33	0.93
1:A:508:SER:HB3	1:A:516:GLN:HG3	1.52	0.92
1:A:211:ALA:HA	3:A:2046:HOH:O	1.70	0.91
1:A:188:LEU:HD11	1:A:206:VAL:HG11	1.54	0.90
1:A:601:ARG:HH21	1:A:619:ASN:HD21	1.20	0.86
1:A:478:ILE:HG23	1:A:491:PHE:HB3	1.58	0.85
1:A:90:LEU:HD22	1:A:94:LEU:HD22	1.59	0.85
1:A:195:ASN:HD22	1:A:196:PRO:HD2	1.42	0.85
1:A:158:TRP:CD1	1:A:168:GLN:HA	2.13	0.83
1:A:177:VAL:HG11	1:A:220:VAL:HG21	1.60	0.83
1:A:449:ASN:ND2	1:A:451:THR:H	1.78	0.82
1:A:614:LEU:HG	1:A:642:ASN:ND2	1.95	0.82
1:A:535:THR:HB	1:A:584:GLN:HG3	1.62	0.81
1:A:431:ASN:H	1:A:431:ASN:HD22	1.27	0.80
1:A:442:LYS:HD2	3:A:2146:HOH:O	1.79	0.80
1:A:121:THR:HG22	1:A:205:LEU:HD12	1.67	0.76
1:A:377:ASN:HD21	1:A:466:THR:HB	1.50	0.76
1:A:101:ILE:HB	1:A:102:PRO:HD3	1.67	0.76
1:A:127:LYS:HB3	1:A:201:TYR:CZ	2.21	0.76
1:A:438:ASN:HD21	1:A:516:GLN:H	1.32	0.76
1:A:204:ILE:HG21	3:A:2064:HOH:O	1.84	0.76
1:A:462:SER:O	1:A:464:GLN:N	2.20	0.75
1:A:645:LYS:H	1:A:645:LYS:CE	1.99	0.74
1:A:195:ASN:HD22	1:A:196:PRO:CD	1.99	0.74
1:A:124:ILE:HD11	1:A:295:TYR:HB2	1.69	0.74
1:A:124:ILE:HG21	3:A:2075:HOH:O	1.88	0.74
1:A:431:ASN:N	1:A:431:ASN:HD22	1.85	0.74
1:A:614:LEU:HG	1:A:642:ASN:HD21	1.53	0.73
1:A:506:SER:HB3	3:A:2121:HOH:O	1.87	0.73
1:A:329:GLU:HB3	3:A:2090:HOH:O	1.89	0.72
1:A:601:ARG:HH21	1:A:619:ASN:ND2	1.87	0.72
1:A:158:TRP:NE1	1:A:168:GLN:HG2	1.96	0.71
1:A:614:LEU:N	1:A:614:LEU:HD12	2.06	0.71
1:A:616:MET:HG3	3:A:2209:HOH:O	1.90	0.71
1:A:645:LYS:N	1:A:645:LYS:HE2	1.99	0.70
1:A:491:PHE:HB2	1:A:492:PRO:HD3	1.71	0.70
1:A:178:HIS:O	1:A:182:GLN:HG3	1.92	0.70
1:A:425:ASN:HB3	1:A:444:ASP:HB2	1.71	0.70
1:A:93:ALA:O	1:A:97:PHE:HB2	1.92	0.70
1:A:200:ASP:O	1:A:204:ILE:HG23	1.91	0.69

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:GLN:HG3	3:A:2211:HOH:O	1.93	0.68
1:A:217:HIS:HD2	1:A:260:TYR:OH	1.77	0.67
1:A:69:GLU:O	1:A:69:GLU:HG2	1.92	0.67
1:A:168:GLN:HB2	3:A:2027:HOH:O	1.94	0.67
1:A:449:ASN:HD22	1:A:449:ASN:C	1.99	0.66
1:A:223:GLN:NE2	1:A:227:PHE:HB2	2.10	0.64
1:A:482:ARG:HD2	1:A:483:GLU:H	1.62	0.64
1:A:140:ILE:HD11	3:A:2040:HOH:O	1.96	0.64
1:A:195:ASN:ND2	1:A:196:PRO:HD2	2.11	0.64
1:A:171:ARG:O	1:A:175:GLN:HG3	1.97	0.64
1:A:381:THR:HG23	1:A:403:ASN:O	1.98	0.64
1:A:122:LYS:HA	1:A:205:LEU:HD11	1.81	0.63
1:A:204:ILE:HD13	3:A:2064:HOH:O	1.99	0.62
1:A:601:ARG:NH2	1:A:619:ASN:HD21	1.96	0.62
1:A:353:LEU:HD22	1:A:519:THR:HG23	1.80	0.62
1:A:159:GLU:HG3	1:A:160:ASN:H	1.65	0.61
1:A:535:THR:CB	1:A:584:GLN:HG3	2.30	0.61
1:A:627:TYR:HB3	1:A:668:LEU:HD11	1.82	0.61
1:A:133:TYR:CZ	1:A:193:PRO:HG3	2.37	0.60
1:A:543:ALA:HB2	1:A:669:ILE:HG22	1.84	0.60
1:A:426:VAL:HG23	3:A:2152:HOH:O	2.02	0.60
1:A:69:GLU:O	1:A:69:GLU:CG	2.49	0.59
1:A:122:LYS:CA	1:A:205:LEU:HD11	2.32	0.59
1:A:122:LYS:NZ	1:A:129:ILE:HG12	2.17	0.59
1:A:124:ILE:CD1	1:A:295:TYR:HB2	2.33	0.59
1:A:97:PHE:HE2	1:A:216:LEU:HD22	1.68	0.58
1:A:528:ASP:OD2	1:A:532:THR:HG23	2.04	0.58
1:A:415:LEU:HD22	1:A:419:ILE:HG22	1.86	0.58
1:A:159:GLU:CG	1:A:160:ASN:H	2.15	0.58
1:A:377:ASN:HA	1:A:465:ILE:HD12	1.84	0.58
1:A:233:ASN:HB2	3:A:2049:HOH:O	2.04	0.57
1:A:358:HIS:HD2	1:A:359:LEU:O	1.87	0.57
1:A:521:ALA:HB1	3:A:2090:HOH:O	2.05	0.57
1:A:449:ASN:HD22	1:A:450:GLY:N	2.02	0.56
1:A:114:TRP:O	1:A:118:ILE:HG13	2.07	0.55
1:A:76:VAL:HG11	1:A:212:GLN:HE22	1.72	0.55
1:A:477:PRO:HD3	3:A:2001:HOH:O	2.07	0.55
1:A:411:LYS:NZ	1:A:459:THR:O	2.34	0.55
1:A:89:PRO:O	1:A:223:GLN:NE2	2.40	0.54
1:A:578:GLN:HB2	3:A:2224:HOH:O	2.08	0.54
1:A:141:LEU:HD21	1:A:188:LEU:HD22	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:CG2	1:A:205:LEU:HD12	2.37	0.54
1:A:618:LEU:HD23	3:A:2209:HOH:O	2.07	0.54
1:A:120:GLN:O	1:A:124:ILE:HG23	2.07	0.54
1:A:158:TRP:HE1	1:A:168:GLN:CG	2.02	0.54
1:A:453:LEU:HD11	1:A:455:GLU:HG3	1.89	0.54
1:A:158:TRP:HD1	1:A:168:GLN:HA	1.65	0.54
1:A:569:PHE:HE2	1:A:604:ILE:HG22	1.73	0.54
1:A:356:ARG:HD2	3:A:2103:HOH:O	2.08	0.54
1:A:449:ASN:C	1:A:449:ASN:ND2	2.61	0.53
1:A:480:LYS:HE3	3:A:2155:HOH:O	2.08	0.53
1:A:275:ILE:HD13	1:A:291:THR:HG22	1.90	0.53
1:A:340:PRO:HG3	1:A:513:TYR:CD2	2.45	0.53
1:A:524:HIS:HD2	1:A:526:SER:CB	2.22	0.53
1:A:185:ILE:HG23	1:A:210:TYR:CE1	2.44	0.52
1:A:383:HIS:HE1	1:A:506:SER:HB2	1.74	0.52
1:A:431:ASN:N	1:A:431:ASN:ND2	2.55	0.52
1:A:664:ASN:HB2	3:A:2228:HOH:O	2.09	0.52
1:A:204:ILE:HG13	1:A:205:LEU:N	2.23	0.52
1:A:572:HIS:HB3	1:A:657:ASN:ND2	2.25	0.52
1:A:354:THR:O	1:A:505:LYS:HE2	2.10	0.52
1:A:170:VAL:HA	3:A:2030:HOH:O	2.09	0.52
1:A:273:ASN:O	1:A:277:THR:HB	2.10	0.52
1:A:84:PHE:CZ	1:A:312:ASN:HB2	2.45	0.52
1:A:356:ARG:CZ	3:A:2238:HOH:O	2.58	0.52
1:A:431:ASN:H	1:A:431:ASN:ND2	2.03	0.51
1:A:124:ILE:HG13	1:A:125:ILE:N	2.24	0.51
1:A:90:LEU:CD2	1:A:94:LEU:HD22	2.37	0.51
1:A:427:ILE:N	1:A:427:ILE:HD12	2.26	0.51
1:A:294:THR:HG22	3:A:2075:HOH:O	2.10	0.51
1:A:357:PRO:HB2	1:A:555:VAL:O	2.11	0.51
1:A:119:THR:HG22	1:A:123:ASN:HD21	1.77	0.50
1:A:70:LEU:HD23	1:A:120:GLN:NE2	2.26	0.50
1:A:590:ILE:N	3:A:2201:HOH:O	2.44	0.50
1:A:90:LEU:HD12	1:A:90:LEU:N	2.27	0.50
1:A:215:ASN:HD22	1:A:310:PHE:HE2	1.59	0.50
1:A:401:PHE:HB3	3:A:2121:HOH:O	2.11	0.50
1:A:166:ASN:C	1:A:168:GLN:H	2.13	0.50
1:A:382:SER:HB2	1:A:401:PHE:O	2.12	0.50
1:A:119:THR:HG22	1:A:123:ASN:ND2	2.27	0.50
1:A:449:ASN:HD21	1:A:452:ARG:H	1.59	0.50
1:A:159:GLU:HG3	1:A:160:ASN:N	2.26	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:PHE:HB3	1:A:506:SER:HB3	1.94	0.49
1:A:202:TYR:O	1:A:206:VAL:HG23	2.12	0.49
1:A:531:ASN:ND2	1:A:575:ILE:CD1	2.76	0.49
1:A:453:LEU:HD13	1:A:453:LEU:C	2.33	0.49
1:A:318:TYR:HB3	1:A:322:VAL:HG22	1.94	0.48
1:A:195:ASN:HD22	1:A:196:PRO:N	2.12	0.48
1:A:591:ARG:O	1:A:670:ASP:HB3	2.14	0.48
1:A:606:LEU:HG	1:A:656:PHE:CE2	2.48	0.48
1:A:206:VAL:HG12	1:A:206:VAL:O	2.13	0.48
1:A:438:ASN:H	1:A:438:ASN:HD22	1.61	0.48
1:A:173:GLN:HB2	3:A:2030:HOH:O	2.12	0.48
1:A:297:THR:HG23	1:A:330:ILE:HD12	1.96	0.48
1:A:532:THR:HA	1:A:578:GLN:O	2.13	0.48
1:A:165:GLN:HA	1:A:168:GLN:HB3	1.96	0.48
1:A:99:THR:HG23	1:A:481:ARG:HD2	1.95	0.48
1:A:136:ASN:O	1:A:140:ILE:HG13	2.14	0.48
1:A:572:HIS:HA	1:A:656:PHE:O	2.13	0.48
1:A:201:TYR:O	1:A:205:LEU:HB2	2.14	0.47
1:A:616:MET:HG2	1:A:640:PHE:CE2	2.50	0.47
1:A:85:GLY:N	3:A:2009:HOH:O	2.48	0.47
1:A:107:ALA:O	1:A:110:GLN:HG2	2.15	0.47
1:A:614:LEU:HD23	1:A:640:PHE:CB	2.45	0.47
1:A:377:ASN:ND2	1:A:466:THR:HB	2.27	0.46
1:A:475:GLY:C	1:A:476:LEU:HD22	2.35	0.46
1:A:133:TYR:CE2	1:A:193:PRO:HG3	2.50	0.46
1:A:188:LEU:HD11	1:A:206:VAL:CG1	2.34	0.46
1:A:169:ASP:O	1:A:172:THR:HG22	2.16	0.46
1:A:393:ASN:C	1:A:393:ASN:HD22	2.19	0.46
1:A:614:LEU:HD23	1:A:640:PHE:HB2	1.96	0.46
1:A:87:THR:O	1:A:87:THR:HG23	2.16	0.46
1:A:228:GLU:OE2	1:A:231:LEU:HD12	2.16	0.46
1:A:588:ILE:HG13	1:A:640:PHE:CD1	2.50	0.46
1:A:150:THR:HG22	1:A:154:HIS:CD2	2.51	0.46
1:A:368:PHE:HB3	1:A:380:PHE:CD2	2.51	0.46
1:A:602:ALA:HA	1:A:660:ASP:CG	2.36	0.45
1:A:452:ARG:CZ	1:A:454:LEU:HD21	2.46	0.45
1:A:363:LEU:HD21	1:A:366:LEU:HD13	1.99	0.45
1:A:429:LEU:HD21	1:A:465:ILE:HD11	1.99	0.44
1:A:449:ASN:ND2	1:A:452:ARG:H	2.14	0.44
1:A:618:LEU:HD23	1:A:638:LEU:HD12	1.99	0.44
1:A:355:ARG:HD2	1:A:503:PHE:CD2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ILE:HG13	1:A:640:PHE:HD1	1.83	0.44
1:A:195:ASN:HB3	1:A:198:ASP:HB2	2.00	0.44
1:A:196:PRO:O	1:A:199:CYS:HB3	2.17	0.44
1:A:234:ASN:HA	3:A:2050:HOH:O	2.16	0.44
1:A:254:THR:HG23	3:A:2216:HOH:O	2.17	0.44
1:A:363:LEU:HD21	1:A:366:LEU:CD1	2.48	0.44
1:A:416:ALA:HB1	3:A:2129:HOH:O	2.17	0.44
1:A:524:HIS:HD2	1:A:526:SER:HB3	1.81	0.44
1:A:408:ASP:N	3:A:2126:HOH:O	2.51	0.44
1:A:480:LYS:CE	3:A:2155:HOH:O	2.65	0.44
1:A:108:GLN:CD	1:A:108:GLN:N	2.71	0.44
1:A:125:ILE:HD13	1:A:204:ILE:HD11	1.99	0.44
1:A:126:LYS:HE2	3:A:2021:HOH:O	2.17	0.44
1:A:593:ALA:HB3	1:A:668:LEU:HB2	1.98	0.44
1:A:661:VAL:O	1:A:663:THR:N	2.50	0.44
1:A:125:ILE:CD1	1:A:204:ILE:HD11	2.47	0.44
1:A:670:ASP:OD2	1:A:671:LYS:HG2	2.18	0.44
1:A:405:ASN:HD22	1:A:408:ASP:HB3	1.83	0.44
1:A:453:LEU:CD1	1:A:455:GLU:HG3	2.48	0.44
1:A:272:LEU:HG	1:A:292:TYR:CZ	2.53	0.43
1:A:491:PHE:CB	1:A:492:PRO:HD3	2.45	0.43
1:A:620:PRO:HG3	3:A:2204:HOH:O	2.18	0.43
1:A:90:LEU:HD21	1:A:159:GLU:HB3	2.00	0.43
1:A:159:GLU:CG	1:A:160:ASN:N	2.81	0.43
1:A:528:ASP:HA	1:A:529:PRO:HD3	1.85	0.43
1:A:166:ASN:C	1:A:168:GLN:N	2.72	0.43
1:A:401:PHE:CZ	2:A:1680:MPD:H11	2.54	0.43
1:A:417:THR:HG21	1:A:530:LYS:NZ	2.33	0.43
1:A:223:GLN:O	1:A:223:GLN:NE2	2.51	0.43
1:A:294:THR:O	1:A:298:LYS:HG2	2.18	0.43
1:A:418:ASN:HA	1:A:420:TYR:CZ	2.53	0.43
1:A:465:ILE:HG12	1:A:469:VAL:HG11	1.99	0.43
1:A:524:HIS:CD2	1:A:526:SER:HB3	2.52	0.43
1:A:588:ILE:HG12	1:A:606:LEU:HD11	2.00	0.43
1:A:151:TYR:HA	1:A:173:GLN:CG	2.49	0.42
1:A:217:HIS:CE1	1:A:221:LEU:HD11	2.54	0.42
1:A:333:VAL:HG23	1:A:334:LEU:N	2.33	0.42
1:A:409:LYS:HE2	1:A:409:LYS:HB3	1.86	0.42
1:A:449:ASN:HD21	1:A:451:THR:H	1.60	0.42
1:A:157:THR:HG22	1:A:157:THR:O	2.19	0.42
1:A:148:ILE:HD11	1:A:181:PHE:CZ	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:PRO:O	1:A:377:ASN:HB2	2.18	0.42
1:A:536:HIS:O	1:A:537:LEU:HB3	2.19	0.42
1:A:569:PHE:CE2	1:A:604:ILE:HG22	2.54	0.42
1:A:608:ILE:CG2	1:A:611:VAL:HB	2.48	0.42
1:A:528:ASP:OD1	1:A:529:PRO:HD2	2.20	0.42
1:A:630:LEU:HD11	1:A:668:LEU:HD12	2.01	0.42
1:A:503:PHE:HZ	2:A:1680:MPD:HM2	1.85	0.42
1:A:614:LEU:N	1:A:614:LEU:CD1	2.75	0.42
1:A:74:THR:HA	3:A:2006:HOH:O	2.19	0.42
1:A:172:THR:O	1:A:175:GLN:HB2	2.20	0.42
1:A:159:GLU:OE2	1:A:160:ASN:ND2	2.53	0.41
1:A:670:ASP:CG	1:A:671:LYS:HG2	2.40	0.41
1:A:77:VAL:HB	3:A:2006:HOH:O	2.20	0.41
1:A:185:ILE:HG23	1:A:210:TYR:HE1	1.84	0.41
1:A:369:TYR:CE2	1:A:410:LEU:HD13	2.55	0.41
1:A:422:PHE:CD1	1:A:492:PRO:HB2	2.54	0.41
1:A:614:LEU:HD12	1:A:614:LEU:H	1.84	0.41
1:A:535:THR:HG22	1:A:586:TYR:OH	2.20	0.41
1:A:585:SER:HA	1:A:644:VAL:O	2.21	0.41
1:A:90:LEU:HD23	1:A:155:LEU:HG	2.02	0.41
1:A:70:LEU:HD23	1:A:120:GLN:HE22	1.86	0.41
1:A:399:SER:H	2:A:1680:MPD:H13	1.86	0.41
1:A:245:THR:O	1:A:247:ILE:HG13	2.21	0.41
1:A:310:PHE:N	1:A:311:PRO:CD	2.83	0.41
1:A:467:TYR:N	1:A:467:TYR:CD2	2.87	0.41
1:A:600:THR:HG22	1:A:662:TYR:CD2	2.54	0.41
1:A:356:ARG:O	1:A:357:PRO:C	2.56	0.41
1:A:367:ASN:HB3	1:A:410:LEU:HD11	2.02	0.41
1:A:405:ASN:HB3	3:A:2125:HOH:O	2.21	0.41
1:A:554:LYS:HE3	3:A:2188:HOH:O	2.21	0.41
1:A:482:ARG:CD	1:A:483:GLU:H	2.32	0.41
1:A:401:PHE:HZ	2:A:1680:MPD:H11	1.85	0.41
1:A:482:ARG:HD2	1:A:483:GLU:N	2.34	0.41
1:A:584:GLN:NE2	1:A:678:THR:O	2.54	0.41
1:A:122:LYS:HZ1	1:A:129:ILE:HG12	1.85	0.40
1:A:381:THR:CG2	1:A:403:ASN:O	2.67	0.40
1:A:151:TYR:HA	1:A:173:GLN:HG2	2.03	0.40
1:A:222:ASN:OD1	1:A:226:LYS:HE3	2.21	0.40
1:A:250:TYR:OH	1:A:316:GLY:HA3	2.21	0.40
1:A:423:LEU:O	1:A:446:PHE:HB2	2.21	0.40
1:A:636:GLN:NE2	1:A:636:GLN:HA	2.36	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:O	1:A:505:LYS:HE3	2.21	0.40
1:A:607:SER:O	1:A:609:PRO:HD3	2.21	0.40
1:A:272:LEU:HG	1:A:292:TYR:CE1	2.56	0.40
1:A:418:ASN:C	1:A:419:ILE:HD12	2.42	0.40
1:A:69:GLU:O	1:A:70:LEU:HB2	2.22	0.40

All (1) 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)
1:A:234:ASN:ND2	1:A:234:ASN:ND2[3_555]	2.04	0.16

## 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	592/612 (97%)	537 (91%)	45 (8%)	10 (2%)	9	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	PRO
1	A	463	GLY
1	A	662	TYR
1	A	373	GLN
1	A	491	PHE
1	A	70	LEU
1	A	159	GLU
1	A	196	PRO
1	A	341	TYR
1	A	162	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	539/557 (97%)	507 (94%)	32 (6%)	19 49

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	PHE
1	A	124	ILE
1	A	141	LEU
1	A	161	ASN
1	A	195	ASN
1	A	223	GLN
1	A	228	GLU
1	A	277	THR
1	A	290	ASN
1	A	317	LYS
1	A	322	VAL
1	A	328	ARG
1	A	333	VAL
1	A	366	LEU
1	A	381	THR
1	A	393	ASN
1	A	403	ASN
1	A	405	ASN
1	A	408	ASP
1	A	431	ASN
1	A	438	ASN
1	A	449	ASN
1	A	456	LYS
1	A	482	ARG
1	A	570	LYS
1	A	575	ILE
1	A	588	ILE
1	A	606	LEU
1	A	614	LEU
1	A	628	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	645	LYS
1	A	649	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	120	GLN
1	A	123	ASN
1	A	146	ASN
1	A	152	HIS
1	A	154	HIS
1	A	160	ASN
1	A	173	GLN
1	A	175	GLN
1	A	195	ASN
1	A	215	ASN
1	A	217	HIS
1	A	223	GLN
1	A	282	ASN
1	A	290	ASN
1	A	312	ASN
1	A	358	HIS
1	A	393	ASN
1	A	396	GLN
1	A	403	ASN
1	A	405	ASN
1	A	431	ASN
1	A	438	ASN
1	A	449	ASN
1	A	524	HIS
1	A	619	ASN
1	A	636	GLN
1	A	657	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	MPD	A	1680	-	7,7,7	0.90	0	9,10,10	0.47	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	MPD	A	1680	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1680	MPD	C1-C2-C3-C4
2	A	1680	MPD	CM-C2-C3-C4
2	A	1680	MPD	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1680	MPD	4	0

## 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 [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	595/612 (97%)	0.07	21 (3%) 44 34	7, 31, 59, 81	51 (8%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ASN	7.5
1	A	89	PRO	6.5
1	A	161	ASN	6.4
1	A	245	THR	6.3
1	A	90	LEU	3.9
1	A	167	THR	3.6
1	A	172	THR	3.1
1	A	484	GLU	3.1
1	A	170	VAL	3.0
1	A	177	VAL	2.9
1	A	483	GLU	2.8
1	A	234	ASN	2.7
1	A	94	LEU	2.5
1	A	88	THR	2.5
1	A	246	ALA	2.5
1	A	86	PHE	2.4
1	A	492	PRO	2.3
1	A	71	SER	2.2
1	A	502	SER	2.2
1	A	171	ARG	2.1
1	A	403	ASN	2.1

### 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 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. 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	MPD	A	1680	8/8	0.83	0.29	30,33,35,37	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.