



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 09:56 PM EST

PDB ID : 1OGG  
Title : chitinase b from serratia marcescens mutant d142n in complex with inhibitor allosamidin  
Authors : Vaaje-Kolstad, G.; Houston, D.R.; Rao, F.V.; Peter, M.G.; Synstad, B.; van Aalten, D.M.F.; Eijsink, V.G.H.  
Deposited on : 2003-04-30  
Resolution : 1.97 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

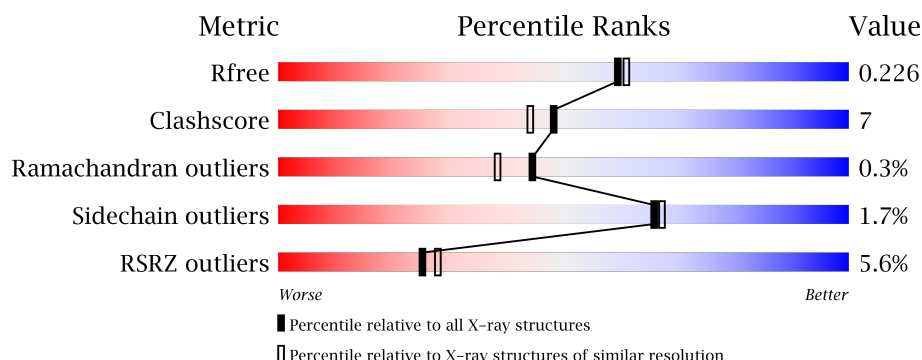
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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	499	<div> <div>7%</div> <div>83%</div> <div>15%</div> </div>
1	B	499	<div> <div>4%</div> <div>88%</div> <div>11%</div> </div>

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
4	GOL	A	1502	-	-	-	X
4	GOL	A	1503	-	-	-	X
4	GOL	A	1504	-	-	-	X
4	GOL	B	1504	-	-	X	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8811 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.

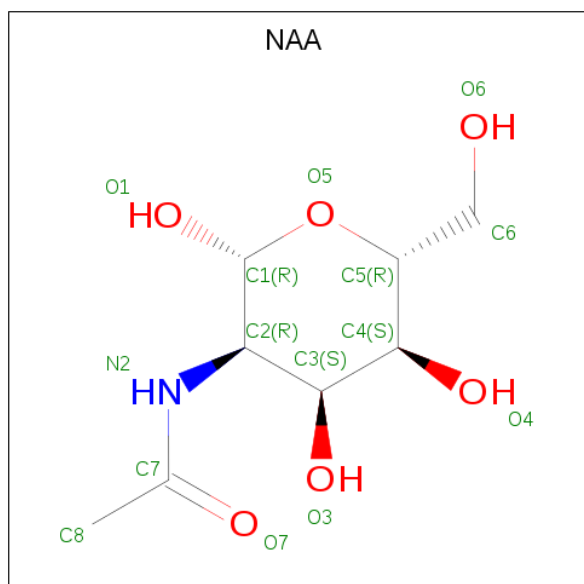
- Molecule 1 is a protein called CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	23	1	1
			3904	2497	661	732	14			
1	B	497	Total	C	N	O	S	12	2	0
			3919	2505	663	737	14			

There are 4 discrepancies between the modelled and reference sequences:

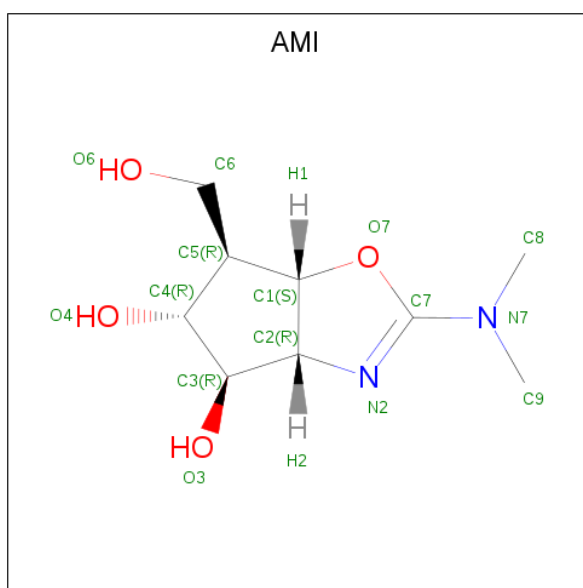
Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASN	ASP	engineered mutation	UNP P11797
B	142	ASN	ASP	engineered mutation	UNP P11797
A	498	VAL	LEU	conflict	UNP P11797
B	498	VAL	LEU	conflict	UNP P11797

- Molecule 2 is N-ACETYL-D-ALLOSAMINE (three-letter code: NAA) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALLOSAMIZOLINE (three-letter code: AMI) (formula:  $C_9H_{16}N_2O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	9	2	4		
3	B	1	Total	C	N	O	0	0
			15	9	2	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

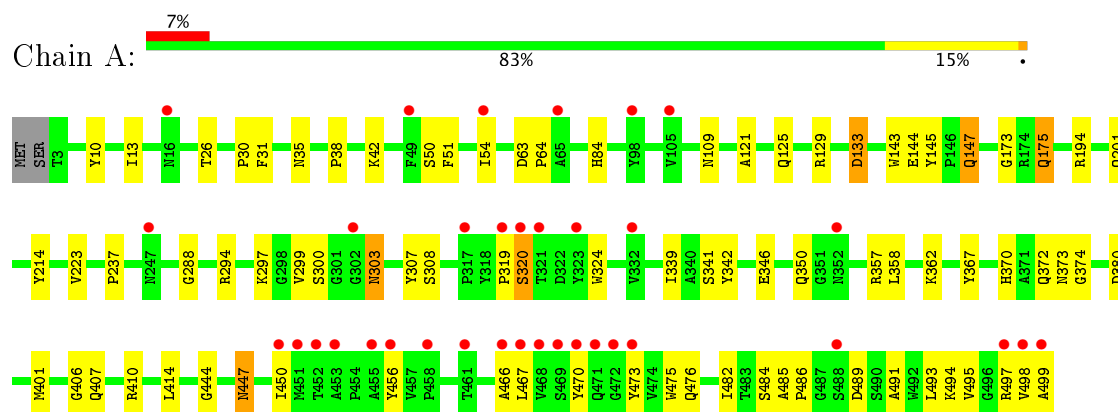
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	386	Total	O	0	0
			386	386		
6	B	475	Total	O	0	0
			475	475		

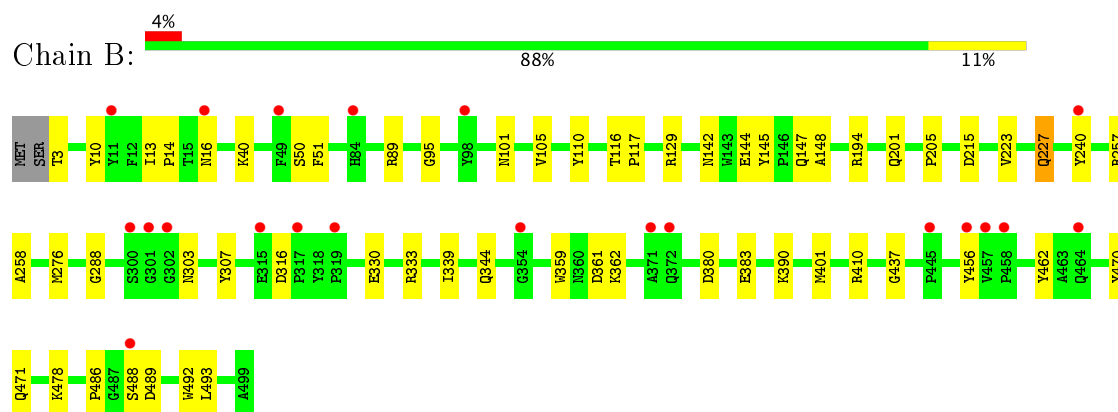
### 3 Residue-property plots [i](#)

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: CHITINASE B



#### • Molecule 1: CHITINASE B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.87Å 104.74Å 186.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.76 – 1.97 25.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.1 (24.76-1.97) 95.2 (25.00-1.97)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 1.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.198 , 0.238 0.186 , 0.226	Depositor DCC
$R_{free}$ test set	732 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8811	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: AMI, GOL, NAA, SO4

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	0.54	0/4019	0.68	0/5478
1	B	57.27	2/4038 (0.0%)	1.12	6/5502 (0.1%)
All	All	40.55	2/8057 (0.0%)	0.92	6/10980 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361[A]	ASP	CA-CB	2573.25	58.15	1.53
1	B	361[B]	ASP	CA-CB	2573.25	58.15	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361[A]	ASP	CB-CA-C	-32.56	45.27	110.40
1	B	361[B]	ASP	CB-CA-C	-32.56	45.27	110.40
1	B	361[A]	ASP	CA-CB-CG	-27.11	53.76	113.40
1	B	361[B]	ASP	CA-CB-CG	-27.11	53.76	113.40
1	B	361[A]	ASP	N-CA-CB	-17.53	79.04	110.60
1	B	361[B]	ASP	N-CA-CB	-17.53	79.04	110.60

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	3904	0	3739	65	0
1	B	3919	0	3752	41	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
3	A	15	0	15	2	0
3	B	15	0	15	2	0
4	A	18	0	24	2	0
4	B	18	0	24	6	0
5	A	5	0	0	0	0
6	A	386	0	0	5	0
6	B	475	0	0	10	0
All	All	8811	0	7619	107	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 (107) 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:444:GLY:H	1:A:447:ASN:HD21	1.08	0.95
1:A:294:ARG:NH1	1:A:339:ILE:HD11	1.84	0.91
1:A:175:GLN:H	1:A:175:GLN:HE21	1.20	0.88
1:B:330:GLU:HA	1:B:333[B]:ARG:NH2	1.89	0.85
1:B:89:ARG:HH12	4:B:1504:GOL:H11	1.44	0.81
1:A:444:GLY:H	1:A:447:ASN:ND2	1.79	0.79
1:A:175:GLN:H	1:A:175:GLN:NE2	1.84	0.75
1:B:129:ARG:HD2	6:B:2167:HOH:O	1.87	0.74
1:B:330:GLU:HA	1:B:333[B]:ARG:HH22	1.54	0.73
1:A:35:ASN:HD21	1:A:410:ARG:HH11	1.38	0.72
1:B:330:GLU:H	1:B:344:GLN:HE21	1.39	0.71
1:B:478:LYS:HE2	1:B:493:LEU:HB2	1.72	0.69
1:B:14:PRO:HB2	1:B:16:ASN:OD1	1.93	0.68
1:A:201:GLN:HG3	6:A:2219:HOH:O	1.95	0.67
1:A:194:ARG:HH21	4:A:1503:GOL:H32	1.58	0.67
6:A:2171:HOH:O	1:B:489:ASP:HB3	1.96	0.65
1:A:299:VAL:HG23	1:A:308:SER:HB3	1.79	0.65
1:A:35:ASN:ND2	1:A:410:ARG:HH11	1.94	0.64
1:A:450:ILE:HG23	1:A:499:ALA:N	2.13	0.64
1:B:89:ARG:NH1	4:B:1504:GOL:H11	2.13	0.63
1:B:89:ARG:HH22	4:B:1504:GOL:C2	2.12	0.62
1:B:201:GLN:HG3	6:B:2239:HOH:O	1.99	0.62
1:A:121:ALA:O	1:A:125[A]:GLN:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:VAL:HG12	1:A:374:GLY:C	2.20	0.61
1:B:257:ARG:HG3	6:B:2279:HOH:O	2.01	0.61
1:B:488:SER:HA	6:B:2456:HOH:O	2.01	0.61
1:B:330:GLU:H	1:B:344:GLN:NE2	1.99	0.60
1:A:299:VAL:HG12	1:A:374:GLY:O	2.01	0.60
1:A:447:ASN:HD22	1:A:447:ASN:H	1.48	0.60
1:B:40:LYS:NZ	6:B:2063:HOH:O	2.20	0.58
1:B:205:PRO:HB3	6:B:2093:HOH:O	2.04	0.58
1:A:346:GLU:O	1:A:350:GLN:HG2	2.03	0.58
1:A:450:ILE:HD12	1:A:499:ALA:N	2.20	0.56
1:B:470:TYR:CD2	1:B:471:GLN:HG3	2.41	0.55
1:B:3:THR:N	6:B:2002:HOH:O	2.39	0.55
1:A:143:TRP:O	1:A:145:TYR:HA	2.06	0.55
1:A:147:GLN:NE2	1:A:194:ARG:CZ	2.70	0.54
1:A:484:SER:HB3	1:A:489:ASP:HB2	1.90	0.54
1:B:89:ARG:HH12	4:B:1504:GOL:C1	2.17	0.54
1:A:447:ASN:HD22	1:A:447:ASN:N	2.05	0.54
1:A:372:GLN:HG2	1:A:373:ASN:OD1	2.09	0.53
1:A:444:GLY:N	1:A:447:ASN:HD21	1.91	0.53
1:B:105:VAL:HG13	6:B:2139:HOH:O	2.09	0.52
1:A:482:ILE:HD12	1:A:491:ALA:CB	2.39	0.52
1:B:215:ASP:H	1:B:227:GLN:HE21	1.57	0.51
1:A:223:VAL:CG2	1:A:307:TYR:HA	2.41	0.51
1:A:175:GLN:N	1:A:175:GLN:HE21	1.99	0.51
1:B:456:TYR:CE1	1:B:462:TYR:HE2	2.29	0.51
1:A:484:SER:HB2	1:B:147:GLN:HE22	1.75	0.51
1:A:450:ILE:HD11	1:A:497:ARG:NH1	2.26	0.50
1:A:362:LYS:NZ	6:A:2309:HOH:O	2.44	0.49
1:A:341:SER:HB2	1:A:407:GLN:HB3	1.94	0.49
1:A:493:LEU:O	1:A:495:VAL:HG13	2.12	0.49
1:B:390:LYS:HE3	6:B:2419:HOH:O	2.11	0.49
1:A:466:ALA:O	1:A:476:GLN:HA	2.12	0.49
1:A:144:GLU:HA	1:A:145:TYR:CG	2.48	0.49
1:A:223:VAL:HG11	1:A:237:PRO:HB3	1.96	0.48
1:A:223:VAL:HG12	6:A:2234:HOH:O	2.12	0.48
1:A:63:ASP:OD1	1:A:64:PRO:HD2	2.14	0.48
1:B:215:ASP:H	1:B:227:GLN:NE2	2.12	0.48
4:B:1503:GOL:H32	6:B:2469:HOH:O	2.15	0.47
1:A:129:ARG:O	1:A:133:ASP:HB2	2.14	0.47
1:A:38:PRO:O	1:A:42:LYS:HG3	2.15	0.47
1:A:370:HIS:CE1	1:A:372:GLN:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:HH22	4:B:1504:GOL:H2	1.78	0.46
1:B:362:LYS:HD3	1:B:437:GLY:HA2	1.96	0.46
1:A:294:ARG:CZ	1:A:339:ILE:HD11	2.45	0.46
1:A:297:LYS:HD3	1:A:324:TRP:CE2	2.51	0.46
1:B:486:PRO:HA	1:B:492:TRP:CD1	2.50	0.45
1:B:95:GLY:HA2	1:B:110:TYR:OH	2.16	0.45
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.82	0.45
1:A:13:ILE:HG23	1:A:13:ILE:O	2.17	0.45
1:A:294:ARG:HG2	1:A:339:ILE:CD1	2.48	0.44
1:A:54:ILE:HG22	1:A:109:ASN:HB3	1.99	0.44
1:A:319:PRO:O	1:A:320:SER:CB	2.65	0.43
1:B:116:THR:HB	1:B:117:PRO:CD	2.48	0.43
1:B:147:GLN:HB3	1:B:194:ARG:HD3	2.00	0.43
1:A:342:TYR:CG	1:A:414:LEU:HD11	2.53	0.43
1:B:223:VAL:HG12	1:B:307:TYR:HA	2.01	0.43
1:A:467:LEU:HA	1:A:475:TRP:O	2.19	0.43
1:A:30:PRO:O	1:A:410:ARG:NH2	2.47	0.43
1:A:214:TYR:OH	3:A:1501:AMI:H82	2.19	0.43
1:A:299:VAL:HG22	1:A:300:SER:N	2.34	0.43
1:B:101:ASN:HA	1:B:144:GLU:O	2.19	0.43
1:B:258:ALA:O	1:B:276:MET:HE1	2.19	0.43
1:B:10:TYR:CE2	3:B:1502:AMI:H91	2.54	0.42
1:B:359:TRP:CH2	1:B:383:GLU:HG2	2.54	0.42
1:A:456:TYR:HB3	1:A:470:TYR:HD1	1.85	0.42
1:B:142:ASN:CG	3:B:1502:AMI:H93	2.39	0.42
1:A:473:TYR:CD2	1:A:494:LYS:HE2	2.55	0.42
1:A:358:LEU:HB2	1:A:367:TYR:CZ	2.54	0.41
1:B:144:GLU:HA	1:B:145:TYR:CG	2.55	0.41
1:A:173:GLY:HA2	1:A:175:GLN:HE22	1.85	0.41
1:B:50:SER:HA	1:B:51:PHE:HA	1.78	0.41
1:A:42:LYS:NZ	1:A:84:HIS:O	2.53	0.41
1:A:485:ALA:HA	1:A:486:PRO:HD3	1.96	0.41
1:B:288:GLY:HA2	1:B:401:MET:O	2.20	0.41
1:A:303:ASN:HA	1:A:303:ASN:HD22	1.63	0.41
1:A:358:LEU:HD12	1:A:367:TYR:CE2	2.55	0.41
1:A:10:TYR:CE2	3:A:1501:AMI:H91	2.55	0.41
1:A:31:PHE:CG	1:A:406:GLY:HA2	2.56	0.41
1:B:13:ILE:HA	1:B:14:PRO:HD3	1.93	0.40
4:A:1504:GOL:H11	6:A:2195:HOH:O	2.21	0.40
1:A:288:GLY:HA2	1:A:401:MET:O	2.21	0.40
1:A:370:HIS:HE1	1:A:372:GLN:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:TRP:CD2	1:A:486:PRO:HB3	2.56	0.40
1:A:50:SER:HA	1:A:51:PHE:HA	1.77	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	496/499 (99%)	485 (98%)	9 (2%)	2 (0%)	38	30
1	B	497/499 (100%)	487 (98%)	9 (2%)	1 (0%)	51	46
All	All	993/998 (100%)	972 (98%)	18 (2%)	3 (0%)	44	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	VAL
1	B	148	ALA
1	A	320	SER

### 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	403/405 (100%)	396 (98%)	7 (2%)	66	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	405/405 (100%)	398 (98%)	7 (2%)	66	67
All	All	808/810 (100%)	794 (98%)	14 (2%)	66	67

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	133	ASP
1	A	147	GLN
1	A	175	GLN
1	A	303	ASN
1	A	380	ASP
1	A	447	ASN
1	B	227	GLN
1	B	240	TYR
1	B	303	ASN
1	B	316	ASP
1	B	339	ILE
1	B	380	ASP
1	B	410	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	109	ASN
1	A	147	GLN
1	A	175	GLN
1	A	303	ASN
1	A	347	GLN
1	A	447	ASN
1	A	464	GLN
1	B	35	ASN
1	B	57	ASN
1	B	112	ASN
1	B	147	GLN
1	B	180	GLN
1	B	227	GLN
1	B	273	GLN
1	B	303	ASN
1	B	344	GLN

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Mol	Chain	Res	Type
1	B	394	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAA	A	1499	2	14,14,15	0.92	1 (7%)	15,19,21	0.64	0
2	NAA	A	1500	3,2	14,14,15	1.00	0	15,19,21	0.97	1 (6%)
3	AMI	A	1501	2	14,16,16	1.18	1 (7%)	18,24,24	2.27	6 (33%)
4	GOL	A	1502	-	5,5,5	0.31	0	5,5,5	0.19	0
4	GOL	A	1503	-	5,5,5	0.44	0	5,5,5	0.12	0
4	GOL	A	1504	-	5,5,5	0.42	0	5,5,5	0.24	0
5	SO4	A	1505	-	4,4,4	0.37	0	6,6,6	0.12	0
2	NAA	B	1500	2	14,14,15	1.00	1 (7%)	15,19,21	0.77	0
2	NAA	B	1501	3,2	14,14,15	0.98	0	15,19,21	0.90	0
3	AMI	B	1502	2	14,16,16	1.07	2 (14%)	18,24,24	2.37	5 (27%)
4	GOL	B	1503	-	5,5,5	0.32	0	5,5,5	0.25	0
4	GOL	B	1504	-	5,5,5	0.37	0	5,5,5	0.24	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	1506	-	5,5,5	0.43	0	5,5,5	0.12	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	NAA	A	1499	2	-	0/6/23/26	0/1/1/1
2	NAA	A	1500	3,2	-	0/6/23/26	0/1/1/1
3	AMI	A	1501	2	-	0/6/34/34	0/2/2/2
4	GOL	A	1502	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1503	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1504	-	-	0/4/4/4	0/0/0/0
5	SO4	A	1505	-	-	0/0/0/0	0/0/0/0
2	NAA	B	1500	2	-	0/6/23/26	0/1/1/1
2	NAA	B	1501	3,2	-	0/6/23/26	0/1/1/1
3	AMI	B	1502	2	-	0/6/34/34	0/2/2/2
4	GOL	B	1503	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1504	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1506	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1502	AMI	C2-N2	-2.28	1.45	1.47
2	A	1499	NAA	C1-C2	2.05	1.55	1.52
3	B	1502	AMI	C7-N2	2.40	1.33	1.29
2	B	1500	NAA	C1-C2	2.43	1.55	1.52
3	A	1501	AMI	C7-N2	2.63	1.33	1.29

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1502	AMI	C5-C4-C3	-5.24	97.99	103.57
3	A	1501	AMI	O7-C7-N2	-4.64	114.73	117.70
3	B	1502	AMI	O7-C7-N2	-4.41	114.88	117.70
3	A	1501	AMI	C5-C4-C3	-4.08	99.23	103.57
3	B	1502	AMI	C1-C2-N2	-2.88	101.96	104.49
3	A	1501	AMI	C1-C2-N2	-2.44	102.35	104.49
2	A	1500	NAA	C1-C2-N2	-2.41	106.37	110.49
3	B	1502	AMI	C1-O7-C7	-2.32	106.28	108.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	AMI	C1-O7-C7	-2.26	106.34	108.92
3	A	1501	AMI	C4-C3-C2	2.06	105.43	102.90
3	B	1502	AMI	C2-N2-C7	5.44	110.49	106.31
3	A	1501	AMI	C2-N2-C7	5.47	110.52	106.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	AMI	2	0
4	A	1503	GOL	1	0
4	A	1504	GOL	1	0
3	B	1502	AMI	2	0
4	B	1503	GOL	1	0
4	B	1504	GOL	5	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 ⓘ

### 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	497/499 (99%)	0.36	35 (7%) 17 19	17, 32, 56, 71	7 (1%)
1	B	497/499 (99%)	0.19	21 (4%) 37 40	18, 28, 48, 58	6 (1%)
All	All	994/998 (99%)	0.28	56 (5%) 25 28	17, 30, 52, 71	13 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	ALA	20.1
1	A	498	VAL	6.6
1	A	450	ILE	6.4
1	A	452	THR	4.3
1	B	445	PRO	3.9
1	B	301	GLY	3.8
1	B	317	PRO	3.6
1	A	473	TYR	3.6
1	B	457	VAL	3.4
1	B	371	ALA	3.2
1	B	84	HIS	3.1
1	A	461	THR	3.0
1	A	456	TYR	2.9
1	A	470	TYR	2.8
1	A	451	MET	2.8
1	A	319	PRO	2.8
1	B	488	SER	2.8
1	A	332	VAL	2.8
1	B	456	TYR	2.8
1	B	464	GLN	2.7
1	A	497	ARG	2.7
1	A	458	PRO	2.7
1	A	472	GLY	2.6
1	A	98	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	466	ALA	2.6
1	A	468	VAL	2.6
1	A	471	GLN	2.5
1	A	453	ALA	2.5
1	A	302	GLY	2.5
1	A	105	VAL	2.5
1	B	315	GLU	2.4
1	A	317	PRO	2.4
1	A	455	ALA	2.4
1	A	488	SER	2.3
1	A	321	THR	2.3
1	B	319	PRO	2.3
1	A	16	ASN	2.3
1	A	65	ALA	2.3
1	B	354	GLY	2.3
1	A	323	TYR	2.2
1	B	98	TYR	2.2
1	B	302	GLY	2.2
1	B	16	ASN	2.1
1	A	320	SER	2.1
1	A	49	PHE	2.1
1	A	352	ASN	2.1
1	B	458	PRO	2.1
1	B	11	TYR	2.1
1	A	469	SER	2.1
1	B	49	PHE	2.1
1	B	300	SER	2.1
1	A	247	ASN	2.1
1	B	372	GLN	2.1
1	A	54	ILE	2.0
1	B	240	TYR	2.0
1	A	467	LEU	2.0

## 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. 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(Å <sup>2</sup> )	Q<0.9
4	GOL	B	1504	6/6	0.82	0.24	4.78	51,53,53,54	0
4	GOL	A	1503	6/6	0.80	0.21	2.96	57,60,61,62	0
4	GOL	A	1502	6/6	0.89	0.17	2.71	30,38,41,42	0
4	GOL	A	1504	6/6	0.88	0.17	2.01	52,54,55,55	0
4	GOL	B	1503	6/6	0.93	0.16	1.21	41,44,46,46	0
2	NAA	A	1499	14/15	0.88	0.21	0.78	44,50,54,54	0
2	NAA	B	1500	14/15	0.88	0.18	0.63	42,48,51,53	0
4	GOL	B	1506	6/6	0.93	0.12	-0.01	33,36,37,38	0
3	AMI	B	1502	15/15	0.97	0.10	-0.51	18,21,25,26	0
3	AMI	A	1501	15/15	0.97	0.09	-0.96	22,24,27,30	0
2	NAA	B	1501	14/15	0.97	0.08	-1.38	20,26,28,32	0
2	NAA	A	1500	14/15	0.96	0.08	-1.42	26,29,32,39	0
5	SO4	A	1505	5/5	0.95	0.16	-	86,87,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.