



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:20 AM GMT

PDB ID : 2CBJ  
Title : STRUCTURE OF THE CLOSTRIDIUM PERFRINGENS NAGJ FAMILY 84 GLYCOSIDE HYDROLASE, A HOMOLOGUE OF HUMAN O-GLCNACASE IN COMPLEX WITH PUGNAC  
Authors : Rao, F.V.; Dorfmüller, H.C.; Villa, F.; Allwood, M.; Eggleston, I.M.; Van Aalten, D.M.F.  
Deposited on : 2006-01-05  
Resolution : 2.35 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

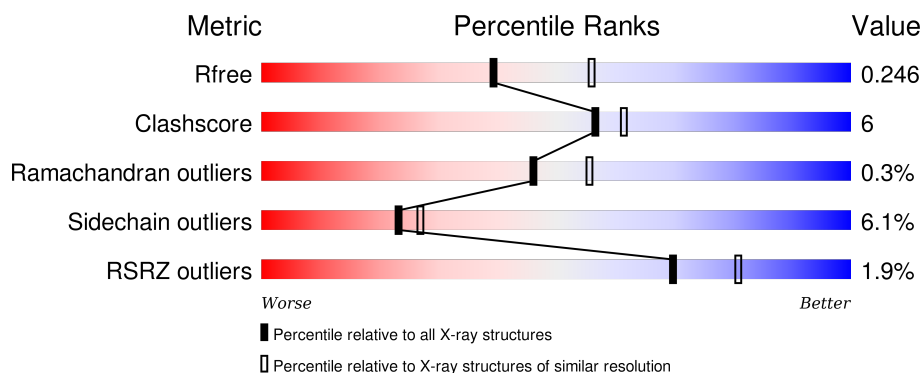
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 82%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>14%</span> <span>...</span> </div> </div>
1	B	594	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 15%, green 82%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>82%</span> <span>15%</span> <span>..</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9589 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.

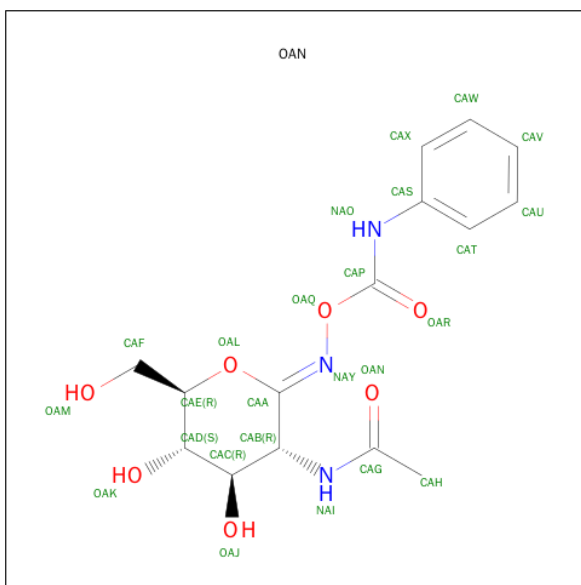
- Molecule 1 is a protein called HYALURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4628	2913	757	941	17			
1	B	585	Total	C	N	O	S	0	0	0
			4629	2913	758	941	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	GLN	LYS	CONFLICT SEE REMARK 9	UNP Q8XL08
A	234	SER	ASN	CONFLICT SEE REMARK 9	UNP Q8XL08
A	244	ASN	ASP	CONFLICT SEE REMARK 9	UNP Q8XL08
A	268	ASP	GLU	CONFLICT SEE REMARK 9	UNP Q8XL08
A	279	THR	ALA	CONFLICT SEE REMARK 9	UNP Q8XL08
A	348	ALA	THR	CONFLICT SEE REMARK 9	UNP Q8XL08
B	196	GLN	LYS	CONFLICT SEE REMARK 9	UNP Q8XL08
B	234	SER	ASN	CONFLICT SEE REMARK 9	UNP Q8XL08
B	244	ASN	ASP	CONFLICT SEE REMARK 9	UNP Q8XL08
B	268	ASP	GLU	CONFLICT SEE REMARK 9	UNP Q8XL08
B	279	THR	ALA	CONFLICT SEE REMARK 9	UNP Q8XL08
B	348	ALA	THR	CONFLICT SEE REMARK 9	UNP Q8XL08

- Molecule 2 is O-(2-ACETAMIDO-2-DEOXY D-GLUCOPYRANOSYLIDENE) AMINO-N-PHENYLCARBAMATE (three-letter code: OAN) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>3</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	15	3	7		
2	B	1	Total	C	N	O	0	0
			25	15	3	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		

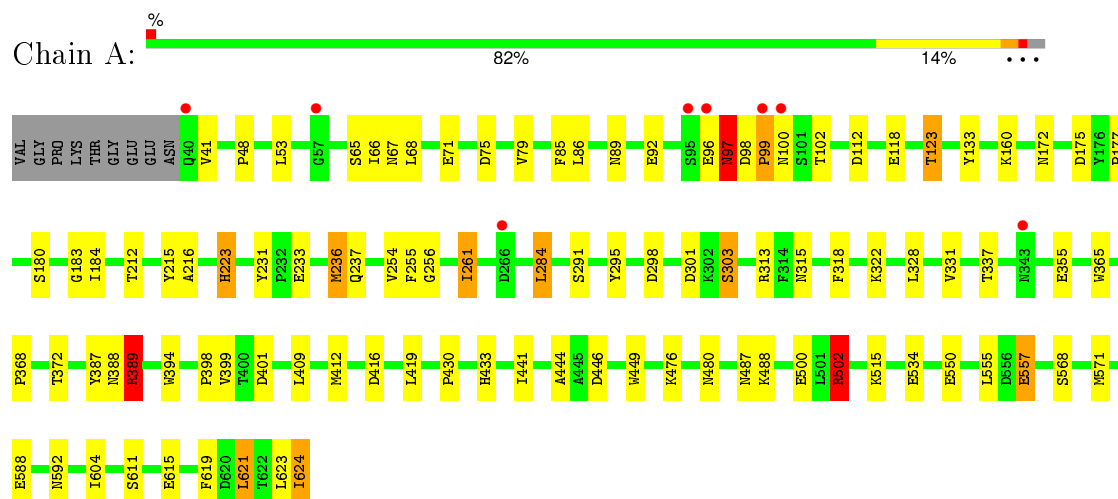
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	137	Total	O	0	0
			137	137		

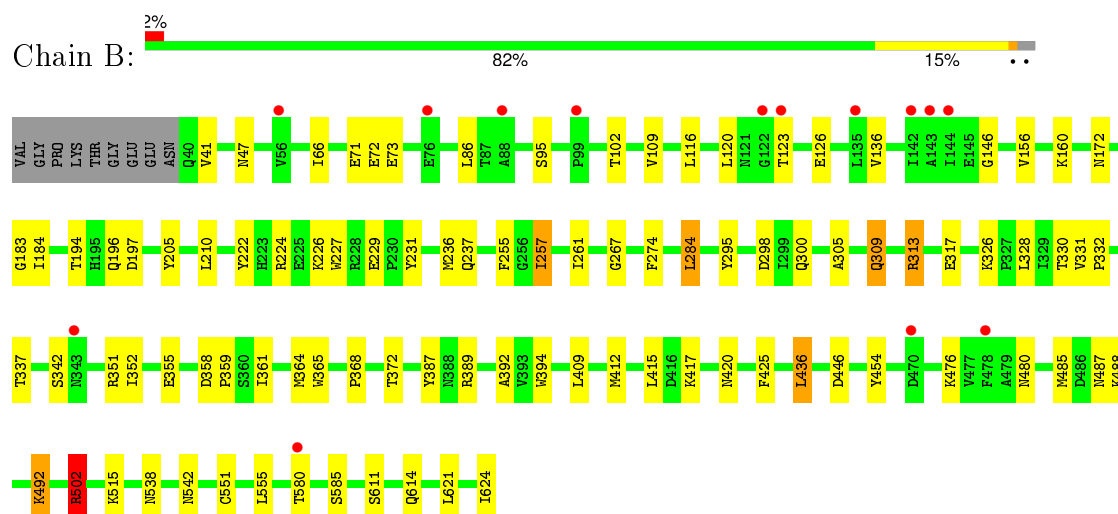
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: HYALURONIDASE



#### • Molecule 1: HYALURONIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.61Å 145.75Å 152.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 19.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.00-2.35) 93.3 (19.99-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.193 , 0.248 0.192 , 0.246	Depositor DCC
$R_{free}$ test set	562 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 29.3	EDS
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 56439 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: OAN, CL

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	0.66	0/4724	0.69	2/6413 (0.0%)
1	B	0.65	1/4725 (0.0%)	0.67	2/6415 (0.0%)
All	All	0.65	1/9449 (0.0%)	0.68	4/12828 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	GLY	C-O	5.49	1.32	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	B	502	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	389	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	502	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	ASN	Peptide
1	A	98	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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	4628	0	4418	62	0
1	B	4629	0	4420	52	0
2	A	25	0	19	1	0
2	B	25	0	19	1	0
3	B	2	0	0	0	0
4	A	143	0	0	2	0
4	B	137	0	0	0	0
All	All	9589	0	8876	109	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 6.

All (109) 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:123:THR:HG21	1:A:172:ASN:HD21	1.05	1.09
1:A:123:THR:HG21	1:A:172:ASN:ND2	1.72	1.03
1:B:305:ALA:O	1:B:309:GLN:HG2	1.61	1.00
1:A:619:PHE:HE2	1:A:621:LEU:HD13	1.29	0.93
1:A:619:PHE:CE2	1:A:621:LEU:HD13	2.10	0.87
1:B:417:LYS:HE2	1:B:454:TYR:O	1.75	0.87
1:A:215:TYR:O	1:A:223:HIS:HE1	1.62	0.83
1:A:223:HIS:CE1	1:A:256:GLY:O	2.39	0.75
1:B:387:TYR:HD2	1:B:389:ARG:NH1	1.86	0.74
1:A:261:ILE:HD13	1:A:261:ILE:H	1.53	0.73
1:B:502:ARG:HD3	1:B:502:ARG:O	1.87	0.73
1:A:387:TYR:HB3	1:A:389:ARG:HD2	1.72	0.71
1:A:231:TYR:HB2	1:A:236:MET:SD	2.31	0.69
1:B:359:PRO:HA	1:B:389:ARG:HH21	1.58	0.69
1:A:295:TYR:CD2	1:A:331:VAL:HG12	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:TYR:O	1:A:223:HIS:CE1	2.47	0.67
1:A:66:ILE:HG22	1:A:102:THR:HB	1.77	0.66
1:B:156:VAL:O	1:B:160:LYS:HG3	1.98	0.63
1:B:66:ILE:HG22	1:B:102:THR:HB	1.80	0.63
1:B:47:ASN:HD21	1:B:446:ASP:HB2	1.64	0.63
1:A:254:VAL:HG22	1:A:291:SER:HB3	1.80	0.62
2:A:1625:OAN:HAV	1:B:621:LEU:HD23	1.81	0.62
1:A:216:ALA:HA	1:A:223:HIS:CE1	2.35	0.61
1:A:65:SER:HB3	1:A:92:GLU:HB3	1.83	0.60
1:A:75:ASP:O	1:A:79:VAL:HG23	2.01	0.60
1:A:96:GLU:O	1:A:97:ASN:HB2	2.01	0.60
1:A:416:ASP:HB3	1:A:419:LEU:HD13	1.84	0.60
1:A:502:ARG:O	1:A:502:ARG:HD3	2.04	0.58
1:B:352:ILE:HA	1:B:355:GLU:HG2	1.88	0.56
1:A:255:PHE:CE2	1:A:284:LEU:HD13	2.41	0.56
1:B:295:TYR:CD2	1:B:331:VAL:HG12	2.41	0.55
1:A:502:ARG:NH2	1:A:615:GLU:OE2	2.38	0.53
1:A:398:PRO:HD2	1:A:430:PRO:HA	1.89	0.53
1:A:183:GLY:C	1:A:184:ILE:HD12	2.29	0.53
1:B:194:THR:O	1:B:197:ASP:HB2	2.09	0.53
1:A:85:PHE:O	1:A:89:ASN:ND2	2.34	0.53
1:B:387:TYR:HD2	1:B:389:ARG:HH11	1.57	0.53
1:B:502:ARG:C	1:B:502:ARG:HD3	2.25	0.52
1:A:500:GLU:OE1	4:A:2098:HOH:O	2.19	0.52
1:A:67:ASN:OD1	1:A:97:ASN:O	2.28	0.52
1:A:515:LYS:NZ	1:B:298:ASP:HA	2.24	0.52
1:B:227:TRP:HB2	1:B:257:ILE:HD11	1.92	0.51
1:B:47:ASN:ND2	1:B:446:ASP:HB2	2.25	0.51
1:B:255:PHE:CE2	1:B:284:LEU:HD13	2.46	0.50
1:B:487:ASN:O	1:B:488:LYS:HB2	2.11	0.50
1:A:133:TYR:CZ	1:A:175:ASP:HB3	2.47	0.50
1:B:183:GLY:C	1:B:184:ILE:HD12	2.33	0.49
1:A:515:LYS:HZ1	1:B:298:ASP:HA	1.78	0.49
1:A:624:ILE:HG22	1:A:624:ILE:OXT	2.11	0.49
1:A:476:LYS:O	1:A:480:ASN:HB2	2.13	0.49
1:B:351:ARG:O	1:B:355:GLU:HG2	2.13	0.49
1:A:624:ILE:HG21	1:B:224:ARG:HH12	1.76	0.49
1:B:538:ASN:OD1	1:B:542:ASN:ND2	2.46	0.48
1:B:417:LYS:CE	1:B:454:TYR:O	2.57	0.48
1:A:254:VAL:HG22	1:A:291:SER:CB	2.44	0.48
1:B:109:VAL:HG11	1:B:126:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:SER:HA	1:B:614:GLN:HE21	1.77	0.48
1:A:68:LEU:HG	1:A:71:GLU:HG3	1.96	0.48
1:B:476:LYS:O	1:B:480:ASN:HB2	2.14	0.48
1:A:133:TYR:CE2	1:A:175:ASP:HB3	2.48	0.47
1:A:624:ILE:CG2	1:B:224:ARG:HH12	2.27	0.47
1:B:313:ARG:HD3	1:B:317:GLU:OE2	2.15	0.47
1:B:205:TYR:HB3	1:B:210:LEU:HB2	1.97	0.47
1:A:216:ALA:HA	1:A:223:HIS:ND1	2.29	0.47
1:B:387:TYR:HB3	1:B:389:ARG:HG2	1.96	0.46
1:A:96:GLU:O	1:A:97:ASN:CB	2.62	0.46
1:A:261:ILE:H	1:A:261:ILE:CD1	2.26	0.46
1:A:487:ASN:O	1:A:488:LYS:HB2	2.15	0.46
1:A:123:THR:CG2	1:A:172:ASN:HD21	1.99	0.46
1:B:337:THR:HB	1:B:368:PRO:HA	1.97	0.46
1:B:231:TYR:HB2	1:B:236:MET:SD	2.56	0.46
1:A:557:GLU:OE1	1:A:604:ILE:HG22	2.15	0.46
1:B:222:TYR:HB2	1:B:231:TYR:CE1	2.51	0.45
1:A:177:PRO:HB3	1:A:449:TRP:CE3	2.51	0.45
1:B:364:MET:HA	1:B:392:ALA:O	2.16	0.45
1:A:433:HIS:HB3	1:A:550:GLU:OE1	2.16	0.45
1:A:502:ARG:C	1:A:502:ARG:HD3	2.34	0.45
1:A:99:PRO:O	1:A:100:ASN:C	2.55	0.45
1:A:48:PRO:HB3	1:A:446:ASP:HA	1.98	0.45
1:A:184:ILE:HD11	1:A:441:ILE:HG23	1.98	0.44
1:A:298:ASP:HA	1:B:515:LYS:HE2	1.98	0.44
1:B:120:LEU:HD23	1:B:136:VAL:HG23	1.98	0.44
1:B:387:TYR:O	1:B:389:ARG:HG2	2.18	0.44
1:B:226:LYS:HB3	1:B:229:GLU:HG3	1.99	0.44
1:B:368:PRO:HD2	1:B:372:THR:HG21	1.99	0.44
1:A:337:THR:HB	1:A:368:PRO:HA	1.99	0.44
1:A:223:HIS:NE2	1:A:256:GLY:O	2.51	0.43
1:A:301:ASP:OD2	1:A:303:SER:OG	2.35	0.43
1:A:85:PHE:CD1	1:A:160:LYS:HG2	2.53	0.43
1:B:387:TYR:CD2	1:B:389:ARG:NH1	2.75	0.43
1:A:412:MET:HG3	1:A:444:ALA:HA	1.99	0.43
1:B:436:LEU:HD21	1:B:551:CYS:HB3	2.01	0.42
1:B:358:ASP:HB2	1:B:361:ILE:HD12	2.01	0.42
1:B:412:MET:HB3	1:B:415:LEU:HD12	2.01	0.42
1:A:315:ASN:ND2	4:A:2024:HOH:O	2.53	0.42
1:A:215:TYR:HD2	1:A:223:HIS:NE2	2.18	0.42
1:B:274:PHE:CZ	1:B:313:ARG:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PHE:O	1:A:322:LYS:HG3	2.19	0.42
1:B:109:VAL:HG23	1:B:146:GLY:O	2.20	0.41
1:A:568:SER:HA	1:A:571:MET:HE2	2.02	0.41
1:A:183:GLY:HA3	1:A:212:THR:O	2.20	0.41
1:B:330:THR:O	1:B:364:MET:HG3	2.20	0.41
1:A:399:VAL:HG22	1:A:401:ASP:H	1.86	0.41
1:A:53:LEU:HD23	1:A:53:LEU:C	2.40	0.41
1:A:388:ASN:C	1:A:389:ARG:HG3	2.41	0.41
1:B:274:PHE:CE2	1:B:313:ARG:HD2	2.56	0.41
1:B:331:VAL:HA	1:B:332:PRO:HD3	1.97	0.40
1:B:485:MET:O	1:B:492:LYS:HA	2.21	0.40
1:B:298:ASP:OD1	2:B:1625:OAN:HAB	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	583/594 (98%)	555 (95%)	24 (4%)	4 (1%)	26	29
1	B	583/594 (98%)	558 (96%)	25 (4%)	0	100	100
All	All	1166/1188 (98%)	1113 (96%)	49 (4%)	4 (0%)	46	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	97	ASN
1	A	99	PRO
1	A	233	GLU

### 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	500/507 (99%)	471 (94%)	29 (6%)	25	29
1	B	500/507 (99%)	468 (94%)	32 (6%)	22	24
All	All	1000/1014 (99%)	939 (94%)	61 (6%)	23	27

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	112	ASP
1	A	118	GLU
1	A	123	THR
1	A	180	SER
1	A	223	HIS
1	A	236	MET
1	A	237	GLN
1	A	261	ILE
1	A	284	LEU
1	A	303	SER
1	A	313	ARG
1	A	328	LEU
1	A	355	GLU
1	A	365	TRP
1	A	372	THR
1	A	389	ARG
1	A	394	TRP
1	A	409	LEU
1	A	502	ARG
1	A	534	GLU
1	A	555	LEU
1	A	557	GLU
1	A	588	GLU
1	A	592	ASN
1	A	611	SER
1	A	621	LEU

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Mol	Chain	Res	Type
1	A	623	LEU
1	A	624	ILE
1	B	41	VAL
1	B	71	GLU
1	B	72	GLU
1	B	73	GLU
1	B	86	LEU
1	B	95	SER
1	B	116	LEU
1	B	123	THR
1	B	172	ASN
1	B	196	GLN
1	B	237	GLN
1	B	257	ILE
1	B	261	ILE
1	B	284	LEU
1	B	300	GLN
1	B	309	GLN
1	B	313	ARG
1	B	326	LYS
1	B	328	LEU
1	B	342	SER
1	B	365	TRP
1	B	394	TRP
1	B	409	LEU
1	B	420	ASN
1	B	425	PHE
1	B	436	LEU
1	B	492	LYS
1	B	502	ARG
1	B	555	LEU
1	B	580	THR
1	B	585	SER
1	B	624	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	223	HIS
1	B	47	ASN
1	B	201	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	309	GLN
1	B	388	ASN
1	B	420	ASN
1	B	614	GLN

### 5.3.3 RNA [i](#)

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	OAN	A	1625	-	22,26,26	1.25	2 (9%)	22,35,35	1.07	1 (4%)
2	OAN	B	1625	-	22,26,26	1.42	3 (13%)	22,35,35	1.52	3 (13%)

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	OAN	A	1625	-	-	0/12/35/35	0/2/2/2
2	OAN	B	1625	-	-	0/12/35/35	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1625	OAN	CAS-NAO	-3.71	1.34	1.41
2	B	1625	OAN	OAQ-NAY	-2.74	1.37	1.44
2	A	1625	OAN	OAQ-NAY	-2.14	1.39	1.44
2	A	1625	OAN	CAA-NAY	2.77	1.34	1.27
2	B	1625	OAN	CAH-CAG	3.05	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1625	OAN	CAS-NAO-CAP	-5.85	116.91	126.39
2	B	1625	OAN	OAR-CAP-NAO	-2.20	120.92	126.14
2	B	1625	OAN	CAB-NAI-CAG	2.44	125.37	122.12
2	A	1625	OAN	CAF-CAE-CAD	2.52	119.23	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1625	OAN	1	0
2	B	1625	OAN	1	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	585/594 (98%)	-0.23	8 (1%) 78 87	27, 45, 74, 90	14 (2%)
1	B	585/594 (98%)	-0.18	14 (2%) 62 74	26, 46, 80, 98	10 (1%)
All	All	1170/1188 (98%)	-0.20	22 (1%) 70 81	26, 45, 78, 98	24 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	PRO	4.3
1	B	122	GLY	4.2
1	B	343	ASN	3.6
1	A	40	GLN	3.3
1	A	99	PRO	2.9
1	A	96	GLU	2.8
1	B	470	ASP	2.7
1	B	123	THR	2.6
1	B	580	THR	2.5
1	A	95	SER	2.5
1	A	57	GLY	2.3
1	B	56	VAL	2.3
1	A	343	ASN	2.3
1	B	88	ALA	2.2
1	B	478	PHE	2.2
1	B	76	GLU	2.2
1	B	143	ALA	2.2
1	A	266	ASP	2.1
1	B	144	ILE	2.0
1	A	100	ASN	2.0
1	B	142	ILE	2.0
1	B	135	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( $\text{\AA}^2$ )	Q<0.9
2	OAN	B	1625	25/25	0.95	0.14	0.80	22,35,68,70	0
2	OAN	A	1625	25/25	0.95	0.12	0.02	25,37,49,54	0
3	CL	B	1626	1/1	0.93	0.12	-	63,63,63,63	0
3	CL	B	1627	1/1	0.89	0.34	-	59,59,59,59	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.