



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 08:28 am GMT

PDB ID : 1HM0  
Title : CRYSTAL STRUCTURE OF S.PNEUMONIAE N-ACETYLGLUCOSAMINE 1-PHOSPHATE URIDYLTRANSFERASE, GLMU  
Authors : Sulzenbacher, G.; Gal, L.; Peneff, C.; Fassy, F.; Bourne, Y.  
Deposited on : 2000-12-04  
Resolution : 2.30 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  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

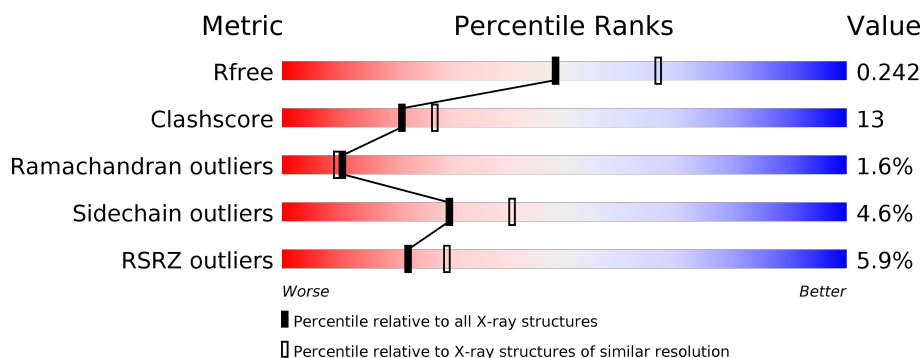
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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	468	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 6%</div> </div> </div>
1	B	468	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6815 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 N-ACETYLGLUCOSAMINE 1-PHOSPHATE URIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3312	2076	568	660	8			
1	B	440	Total	C	N	O	S	0	0	0
			3312	2076	568	660	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	88	Total	O	0	0
			88	88		



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.72Å 92.72Å 280.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.30 39.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.5 (40.00-2.30) 94.5 (39.74-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.207 , 0.244 0.202 , 0.242	Depositor DCC
$R_{free}$ test set	3766 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.467 for -h-k,k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.37% 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: CA

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	0.56	0/3358	0.71	1/4554 (0.0%)
1	B	0.56	0/3358	0.72	1/4554 (0.0%)
All	All	0.56	0/6716	0.72	2/9108 (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	B	370	GLU	N-CA-C	-6.04	94.69	111.00
1	A	370	GLU	N-CA-C	-5.72	95.57	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	3312	0	3311	83	0
1	B	3312	0	3311	89	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	97	0	0	4	0
3	B	88	0	0	3	0
All	All	6815	0	6622	172	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 13.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:HA	1:B:12:LYS:NZ	1.86	0.91
1:B:124:VAL:HA	1:B:176:ASP:OD2	1.81	0.80
1:A:63:LEU:HD23	1:A:63:LEU:H	1.45	0.79
1:A:124:VAL:HA	1:A:176:ASP:OD2	1.86	0.76
1:B:12:LYS:HA	1:B:12:LYS:HZ2	1.51	0.73
1:A:63:LEU:N	1:A:63:LEU:HD23	2.03	0.73
1:A:33:LEU:HD23	1:A:63:LEU:HD12	1.69	0.72
1:B:63:LEU:H	1:B:63:LEU:HD23	1.54	0.71
1:A:124:VAL:HG21	1:A:210:GLU:HB3	1.77	0.66
1:A:106:ILE:HA	1:A:222:GLU:HG3	1.78	0.66
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.60	0.66
1:B:63:LEU:HD23	1:B:63:LEU:N	2.10	0.66
1:B:206:ARG:HH11	1:B:206:ARG:HG2	1.61	0.65
1:B:12:LYS:HZ3	1:B:12:LYS:CA	2.11	0.64
1:A:86:GLU:HB3	1:A:87:PRO:HD3	1.79	0.64
1:B:187:ILE:O	1:B:191:ASN:HB2	1.98	0.63
1:A:82:VAL:HG11	1:A:198:ILE:HD13	1.81	0.63
1:B:86:GLU:HB3	1:B:87:PRO:HD3	1.81	0.63
1:B:12:LYS:HA	1:B:12:LYS:HZ3	1.62	0.62
1:A:62:VAL:HB	1:A:63:LEU:HD23	1.81	0.62
1:B:33:LEU:HD23	1:B:63:LEU:HD12	1.82	0.61
1:A:187:ILE:O	1:A:191:ASN:HB2	2.01	0.61
1:B:124:VAL:HG21	1:B:210:GLU:HB3	1.81	0.61
1:A:191:ASN:ND2	1:A:193:GLN:HB3	2.15	0.61
1:B:12:LYS:N	1:B:12:LYS:HZ3	1.99	0.61
1:B:12:LYS:CA	1:B:12:LYS:NZ	2.63	0.61
1:B:332:ARG:HB3	1:B:333:PRO:CD	2.31	0.60
1:B:72:GLN:HG3	1:B:72:GLN:O	1.99	0.60
1:B:12:LYS:H	1:B:12:LYS:HZ3	1.49	0.60
1:B:191:ASN:ND2	1:B:193:GLN:HB3	2.16	0.59
1:B:431:PRO:HG2	1:B:434:ALA:HB2	1.84	0.59
1:A:206:ARG:HG2	1:A:206:ARG:NH1	2.18	0.59
1:A:31:SER:OG	1:A:34:GLU:HG3	2.02	0.59
1:B:106:ILE:HA	1:B:222:GLU:HG3	1.83	0.59
1:A:10:ALA:O	1:A:11:GLY:O	2.21	0.58
1:B:62:VAL:HB	1:B:63:LEU:HD23	1.84	0.58
1:B:82:VAL:HG11	1:B:198:ILE:HD13	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HG	1:A:206:ARG:HH22	1.68	0.57
1:A:332:ARG:HB3	1:A:333:PRO:CD	2.34	0.57
1:A:72:GLN:O	1:A:72:GLN:HG3	2.05	0.57
1:B:206:ARG:NH1	1:B:206:ARG:HG2	2.20	0.56
1:B:149:VAL:HB	1:B:212:VAL:O	2.04	0.56
1:A:33:LEU:HD23	1:A:63:LEU:CD1	2.36	0.56
1:A:57:GLU:HA	1:A:60:GLU:OE1	2.06	0.56
1:A:419:LEU:HD23	1:A:419:LEU:C	2.26	0.56
1:B:60:GLU:O	1:B:64:ALA:HB2	2.07	0.55
1:A:111:LEU:O	1:A:114:LEU:HB3	2.07	0.55
1:B:227:ASN:HB2	3:B:1039:HOH:O	2.07	0.55
1:A:127:ILE:HD13	1:A:152:ILE:HD11	1.89	0.55
1:B:111:LEU:O	1:B:114:LEU:HB3	2.07	0.55
1:A:195:GLU:H	1:A:195:GLU:CD	2.10	0.54
1:B:21:PRO:HG3	1:B:55:LYS:HB2	1.90	0.54
1:A:149:VAL:HB	1:A:212:VAL:O	2.07	0.54
1:B:419:LEU:C	1:B:419:LEU:HD23	2.28	0.54
1:A:133:ASP:OD1	1:A:166:LYS:NZ	2.42	0.53
1:A:419:LEU:HD23	1:A:420:VAL:N	2.23	0.53
1:A:60:GLU:O	1:A:64:ALA:HB2	2.08	0.53
1:B:195:GLU:CD	1:B:195:GLU:H	2.11	0.53
1:A:168:ILE:HD12	1:A:168:ILE:C	2.30	0.53
1:B:162:GLU:C	1:B:164:GLN:H	2.13	0.53
1:A:162:GLU:C	1:A:164:GLN:H	2.12	0.52
1:A:227:ASN:ND2	3:A:985:HOH:O	2.39	0.52
1:B:151:ARG:HH11	1:B:151:ARG:HG2	1.73	0.52
1:A:21:PRO:HG3	1:A:55:LYS:HB2	1.90	0.52
1:A:78:THR:O	1:A:82:VAL:HG12	2.10	0.52
1:A:57:GLU:O	1:A:61:GLU:N	2.37	0.52
1:B:168:ILE:C	1:B:168:ILE:HD12	2.31	0.51
1:B:57:GLU:O	1:B:61:GLU:N	2.37	0.51
1:B:57:GLU:HA	1:B:60:GLU:OE1	2.10	0.51
1:A:63:LEU:CD2	1:A:63:LEU:H	2.08	0.51
1:B:218:LYS:N	1:B:218:LYS:HD3	2.25	0.51
1:A:431:PRO:HG2	1:A:434:ALA:HB2	1.93	0.50
1:A:332:ARG:HB3	1:A:333:PRO:HD2	1.93	0.50
1:A:178:GLU:O	1:A:182:GLU:HG3	2.12	0.50
1:B:140:ARG:HB3	1:B:165:ILE:HD12	1.94	0.50
1:A:56:ALA:O	1:A:60:GLU:HG3	2.11	0.49
1:A:128:LEU:HB3	1:A:172:THR:HB	1.93	0.49
1:B:183:ALA:O	1:B:187:ILE:HG13	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:THR:O	1:B:161:PHE:N	2.46	0.48
1:B:31:SER:OG	1:B:34:GLU:HG3	2.12	0.48
1:B:332:ARG:HB3	1:B:333:PRO:HD2	1.96	0.48
1:B:127:ILE:HD13	1:B:152:ILE:HD11	1.96	0.48
1:B:66:GLN:O	1:B:67:THR:HB	2.14	0.48
1:B:227:ASN:ND2	3:B:1068:HOH:O	2.46	0.48
1:B:419:LEU:HD23	1:B:420:VAL:N	2.28	0.48
1:A:327:PRO:O	1:A:345:ASN:HA	2.13	0.47
1:A:40:VAL:O	1:A:43:ILE:HG12	2.14	0.47
1:A:159:THR:O	1:A:161:PHE:N	2.47	0.47
1:B:270:PRO:O	1:B:271:GLU:HB2	2.13	0.47
1:A:53:GLY:O	1:A:56:ALA:HB2	2.15	0.47
1:B:150:LEU:HG	1:B:206:ARG:HH22	1.79	0.47
1:A:218:LYS:N	1:A:218:LYS:HD3	2.29	0.46
1:A:62:VAL:CB	1:A:63:LEU:HD23	2.45	0.46
1:A:140:ARG:HB3	1:A:165:ILE:HD12	1.97	0.46
1:B:40:VAL:O	1:B:43:ILE:HG12	2.16	0.46
1:A:395:VAL:HB	1:A:413:GLU:HG3	1.97	0.46
1:A:362:HIS:N	1:A:362:HIS:CD2	2.84	0.46
1:A:227:ASN:HB2	3:A:927:HOH:O	2.15	0.46
1:B:367:GLY:O	1:B:385:ASN:ND2	2.49	0.46
1:B:206:ARG:O	1:B:206:ARG:HD3	2.16	0.46
1:B:395:VAL:HB	1:B:413:GLU:HG3	1.98	0.45
1:B:431:PRO:HG2	1:B:434:ALA:CB	2.47	0.45
1:B:62:VAL:CB	1:B:63:LEU:HD23	2.47	0.45
1:B:218:LYS:CD	1:B:218:LYS:H	2.29	0.45
1:B:178:GLU:O	1:B:182:GLU:HG3	2.16	0.45
1:B:53:GLY:O	1:B:56:ALA:HB2	2.16	0.45
1:A:156:LYS:HG3	1:A:157:ASP:OD1	2.16	0.45
1:A:270:PRO:O	1:A:271:GLU:HB2	2.16	0.45
1:B:6:ILE:HD13	1:B:82:VAL:HG23	1.98	0.45
1:A:191:ASN:HB3	3:A:933:HOH:O	2.17	0.45
1:B:63:LEU:N	1:B:63:LEU:CD2	2.77	0.44
1:A:196:TYR:CD1	1:A:196:TYR:N	2.84	0.44
1:B:196:TYR:CD1	1:B:196:TYR:N	2.86	0.44
1:A:310:THR:O	1:A:327:PRO:HA	2.18	0.44
1:A:67:THR:HG23	1:A:69:PHE:CE1	2.53	0.44
1:A:42:ALA:O	1:A:112:LYS:HD2	2.18	0.44
1:A:66:GLN:O	1:A:67:THR:HB	2.18	0.43
1:A:159:THR:C	1:A:161:PHE:N	2.71	0.43
1:A:432:ALA:O	1:A:433:ASP:HB2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:THR:O	1:B:82:VAL:HG12	2.19	0.43
1:B:361:GLY:C	1:B:362:HIS:CG	2.92	0.43
1:B:86:GLU:HA	1:B:181:PHE:CE1	2.53	0.43
1:B:128:LEU:HB3	1:B:172:THR:HB	1.99	0.43
1:B:327:PRO:O	1:B:345:ASN:HA	2.18	0.43
1:B:389:LYS:HE3	1:B:389:LYS:HB2	1.90	0.43
1:B:441:ARG:HG3	1:B:443:ILE:HD11	2.00	0.43
1:A:206:ARG:O	1:A:206:ARG:HD3	2.19	0.43
1:A:141:ILE:O	1:A:165:ILE:HG21	2.19	0.43
1:B:191:ASN:HB3	3:B:1037:HOH:O	2.18	0.43
1:B:159:THR:C	1:B:161:PHE:N	2.71	0.43
1:B:42:ALA:O	1:B:112:LYS:HD2	2.19	0.43
1:A:132:THR:O	1:A:166:LYS:HG3	2.19	0.42
1:B:10:ALA:O	1:B:11:GLY:O	2.37	0.42
1:B:293:THR:OG1	1:B:310:THR:HA	2.19	0.42
1:A:300:ASP:O	1:A:316:GLU:HA	2.19	0.42
1:B:63:LEU:H	1:B:63:LEU:CD2	2.15	0.42
1:A:412:VAL:HG22	1:A:413:GLU:N	2.34	0.42
1:A:191:ASN:HD21	1:A:193:GLN:HB3	1.81	0.42
1:B:432:ALA:O	1:B:433:ASP:HB2	2.20	0.42
1:A:361:GLY:C	1:A:362:HIS:CG	2.92	0.42
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.84	0.42
1:B:62:VAL:CG1	1:B:63:LEU:HD23	2.49	0.42
1:A:134:ASN:N	1:A:135:PRO:HD3	2.35	0.42
1:B:86:GLU:O	1:B:90:GLU:HB2	2.20	0.42
1:A:269:ALA:HA	1:A:270:PRO:HD3	1.87	0.41
1:B:206:ARG:C	1:B:206:ARG:HD3	2.40	0.41
1:B:412:VAL:HG22	1:B:413:GLU:N	2.36	0.41
1:A:121:HIS:HB3	1:A:211:LYS:HZ1	1.84	0.41
1:A:62:VAL:CG1	1:A:63:LEU:HD23	2.50	0.41
1:A:6:ILE:HD13	1:A:82:VAL:HG23	2.02	0.41
1:A:183:ALA:O	1:A:187:ILE:HG13	2.21	0.41
1:A:394:THR:OG1	1:A:410:ALA:HB2	2.19	0.41
1:A:115:ILE:O	1:A:116:ASP:C	2.59	0.41
1:B:141:ILE:O	1:B:165:ILE:HG21	2.21	0.41
1:B:33:LEU:HD23	1:B:63:LEU:CD1	2.48	0.41
1:A:133:ASP:C	1:A:135:PRO:HD3	2.40	0.41
1:B:151:ARG:NH1	1:B:151:ARG:HG2	2.36	0.41
1:A:13:GLY:N	3:A:984:HOH:O	2.41	0.41
1:B:115:ILE:O	1:B:116:ASP:C	2.58	0.41
1:B:193:GLN:HG2	1:B:194:GLY:N	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:HG2	1:A:151:ARG:HH11	1.84	0.41
1:B:442:GLN:O	1:B:443:ILE:HD13	2.21	0.41
1:B:56:ALA:O	1:B:60:GLU:HG3	2.21	0.41
1:A:138:TYR:HB3	1:A:168:ILE:HB	2.03	0.41
1:B:133:ASP:HA	1:B:166:LYS:HZ2	1.86	0.40
1:A:339:ALA:O	1:A:356:GLU:HB2	2.21	0.40
1:B:154:GLU:O	1:B:158:ALA:HB2	2.22	0.40
1:B:269:ALA:HA	1:B:270:PRO:HD3	1.91	0.40
1:A:218:LYS:CD	1:A:218:LYS:H	2.32	0.40
1:A:55:LYS:O	1:A:58:LEU:HB3	2.22	0.40
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.87	0.40
1:B:67:THR:HG23	1:B:69:PHE:CE1	2.56	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	436/468 (93%)	406 (93%)	23 (5%)	7 (2%)	11	10
1	B	436/468 (93%)	404 (93%)	25 (6%)	7 (2%)	11	10
All	All	872/936 (93%)	810 (93%)	48 (6%)	14 (2%)	11	10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY
1	B	11	GLY
1	A	62	VAL
1	B	62	VAL
1	B	67	THR
1	A	67	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	160	ASP
1	A	163	LYS
1	B	160	ASP
1	B	163	LYS
1	A	61	GLU
1	B	61	GLU
1	B	65	GLY
1	A	65	GLY

### 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	361/386 (94%)	346 (96%)	15 (4%)	32	45
1	B	361/386 (94%)	343 (95%)	18 (5%)	27	37
All	All	722/772 (94%)	689 (95%)	33 (5%)	29	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	63	LEU
1	A	66	GLN
1	A	134	ASN
1	A	157	ASP
1	A	166	LYS
1	A	195	GLU
1	A	196	TYR
1	A	206	ARG
1	A	218	LYS
1	A	318	SER
1	A	345	ASN
1	A	362	HIS
1	A	385	ASN
1	A	390	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	12	LYS
1	B	46	GLU
1	B	63	LEU
1	B	66	GLN
1	B	90	GLU
1	B	133	ASP
1	B	157	ASP
1	B	166	LYS
1	B	195	GLU
1	B	196	TYR
1	B	206	ARG
1	B	218	LYS
1	B	318	SER
1	B	345	ASN
1	B	362	HIS
1	B	385	ASN
1	B	390	ASN
1	B	441	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	95	HIS
1	A	134	ASN
1	A	191	ASN
1	A	277	ASN
1	A	362	HIS
1	A	390	ASN
1	B	54	HIS
1	B	66	GLN
1	B	120	ASN
1	B	191	ASN
1	B	250	ASN
1	B	277	ASN
1	B	362	HIS
1	B	390	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](#)

Of 6 ligands modelled in this entry, 6 are 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 [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	440/468 (94%)	0.31	28 (6%) 19 25	18, 45, 86, 99	0
1	B	440/468 (94%)	0.28	24 (5%) 25 32	18, 46, 86, 99	0
All	All	880/936 (94%)	0.29	52 (5%) 22 29	18, 46, 86, 99	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	HIS	7.3
1	B	66	GLN	5.4
1	B	443	ILE	5.2
1	A	63	LEU	4.8
1	B	54	HIS	4.3
1	A	213	GLY	4.1
1	B	161	PHE	3.7
1	B	194	GLY	3.5
1	B	63	LEU	3.4
1	B	392	TYR	3.4
1	A	197	TYR	3.2
1	A	69	PHE	3.2
1	A	214	ALA	3.2
1	B	62	VAL	3.2
1	B	61	GLU	3.1
1	A	149	VAL	3.0
1	A	192	ALA	2.8
1	B	154	GLU	2.8
1	A	387	ASP	2.7
1	A	162	GLU	2.5
1	A	164	GLN	2.5
1	A	151	ARG	2.5
1	A	184	LEU	2.5
1	B	195	GLU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	159	THR	2.4
1	B	37	PHE	2.4
1	A	116	ASP	2.4
1	A	218	LYS	2.4
1	A	60	GLU	2.4
1	B	68	GLU	2.4
1	B	69	PHE	2.4
1	B	73	SER	2.3
1	B	217	LEU	2.3
1	B	197	TYR	2.3
1	A	154	GLU	2.3
1	B	60	GLU	2.2
1	A	156	LYS	2.2
1	A	161	PHE	2.2
1	A	55	LYS	2.2
1	A	122	LYS	2.1
1	A	388	GLY	2.2
1	B	212	VAL	2.1
1	A	180	LEU	2.1
1	A	67	THR	2.1
1	B	387	ASP	2.1
1	B	389	LYS	2.1
1	A	152	ILE	2.1
1	A	91	GLY	2.1
1	B	86	GLU	2.0
1	A	62	VAL	2.0
1	A	389	LYS	2.0
1	B	149	VAL	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. 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	CA	B	901	1/1	0.31	0.12	57,57,57,57	1
2	CA	A	901	1/1	0.69	0.12	50,50,50,50	1
2	CA	B	903	1/1	0.94	0.24	35,35,35,35	1
2	CA	A	902	1/1	0.97	0.28	34,34,34,34	0
2	CA	B	902	1/1	0.97	0.30	34,34,34,34	0
2	CA	A	903	1/1	0.98	0.31	34,34,34,34	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.