



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:07 AM GMT

PDB ID : 2VZO  
Title : CRYSTAL STRUCTURE OF AMYCOLATOPSIS ORIENTALIS EXO-CHITOSANASE CSXA  
Authors : Lammerts Van Bueren, A.; Ghinet, M.G.; Gregg, K.; Fleury, A.; Brzezinski, R.; Boraston, A.B.  
Deposited on : 2008-08-05  
Resolution : 2.24 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.

---

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

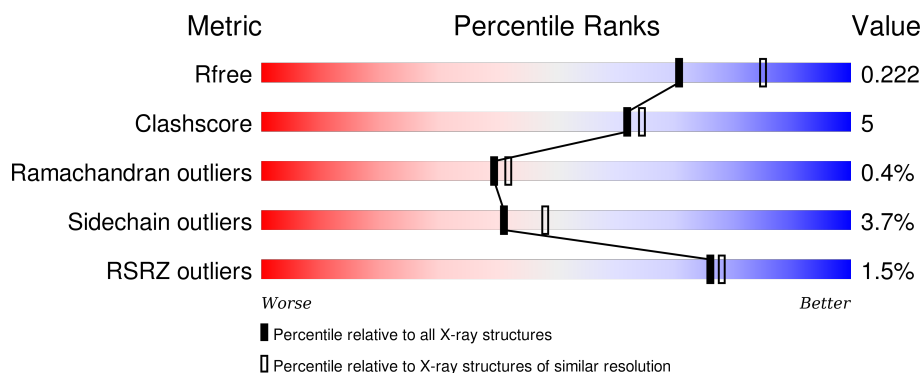
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	1032	<div> <div></div> <div>71% 9% • 18%</div> </div>
1	B	1032	<div> <div></div> <div>72% 8% • 18%</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
3	ACT	A	1906	-	-	-	X
3	ACT	B	1906	-	-	-	X
4	GOL	A	1907	-	-	-	X
4	GOL	B	1907	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13644 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 EXO-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	851	Total	C	N	O	S	9	0	1
			6510	4090	1126	1277	17			
1	B	849	Total	C	N	O	S	0	0	1
			6488	4077	1123	1271	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	GLU	ASP	ENGINEERED MUTATION	UNP Q56F26
A	750	ASN	TRP	CONFLICT	UNP Q56F26
B	469	GLU	ASP	ENGINEERED MUTATION	UNP Q56F26
B	750	ASN	TRP	CONFLICT	UNP Q56F26

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Cd	0	0
			6	6		
2	A	7	Total	Cd	0	0
			7	7		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- 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		

*Continued on next page...*

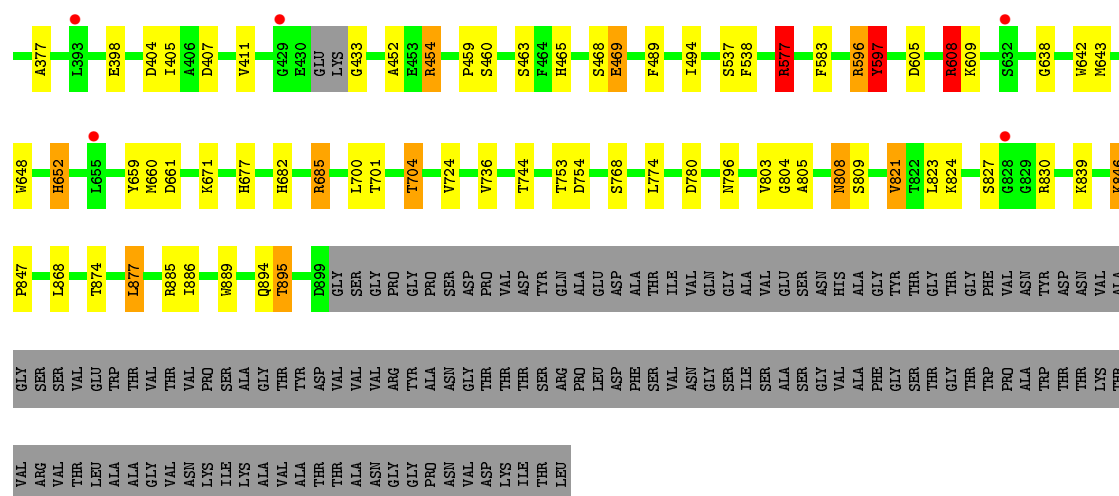
*Continued from previous page...*

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	301	Total	O	0	0
			301	301		
5	B	306	Total	O	0	0
			306	306		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.40 Å   122.03 Å   91.60 Å 90.00°   90.52°   90.00°	Depositor
Resolution (Å)	20.00 – 2.24 39.21 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.24) 99.2 (39.21-2.24)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.24 (at 2.24 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.175   ,   0.223 0.174   ,   0.222	Depositor DCC
$R_{free}$ test set	4527 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36   ,   34.7	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90212 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CD, ACT

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	1.15	2/6673 (0.0%)	0.92	23/9105 (0.3%)
1	B	0.81	0/6650	0.85	24/9074 (0.3%)
All	All	1.00	2/13323 (0.0%)	0.89	47/18179 (0.3%)

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	2	3
1	B	1	3
All	All	3	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	GLU	CA-CB	66.07	2.99	1.53
1	A	430	GLU	CB-CG	12.27	1.75	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	GLU	N-CA-CB	-26.56	62.79	110.60
1	A	431	GLU	CB-CA-C	-21.26	67.88	110.40
1	A	454	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	B	335	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	335	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	B	230	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	A	597	TYR	N-CA-C	8.97	135.21	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	597	TYR	N-CA-C	8.68	134.43	111.00
1	B	454	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	311	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	B	608	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	577	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	454	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	230	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	454	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	577	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	469	GLU	N-CA-C	7.12	130.23	111.00
1	B	222	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	B	608	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	144	LEU	CA-CB-CG	6.91	131.19	115.30
1	A	238	LEU	CA-CB-CG	6.87	131.11	115.30
1	B	577	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	469	GLU	N-CA-C	6.74	129.20	111.00
1	A	577	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	311	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	335	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	596	ARG	C-N-CA	6.15	137.08	121.70
1	A	421	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	335	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	596	ARG	C-N-CA	5.84	136.31	121.70
1	B	144	LEU	CB-CG-CD2	5.60	120.52	111.00
1	B	774	LEU	CA-CB-CG	-5.47	102.72	115.30
1	B	99	LYS	N-CA-C	-5.42	96.36	111.00
1	B	311	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	67	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	774	LEU	CA-CB-CG	-5.38	102.92	115.30
1	B	685	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	596	ARG	N-CA-C	5.18	124.99	111.00
1	B	243	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	407	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	230	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	431	GLU	CA-CB-CG	5.11	124.65	113.40
1	B	596	ARG	N-CA-C	5.11	124.81	111.00
1	A	210	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	378	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	762	ARG	NE-CZ-NH2	-5.01	117.80	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	469	GLU	CA
1	A	597	TYR	CA
1	B	597	TYR	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	SER	Peptide
1	A	596	ARG	Peptide
1	A	98	GLY	Peptide
1	B	468	SER	Peptide
1	B	596	ARG	Peptide
1	B	98	GLY	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	6510	0	6287	69	0
1	B	6488	0	6263	68	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
5	A	301	0	0	9	1
5	B	306	0	0	11	1
All	All	13644	0	12580	137	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 5.

All (137) 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:109:MET:CE	1:B:368:PHE:HE1	1.50	1.22

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:CE	1:B:368:PHE:CE1	2.29	1.14
1:B:109:MET:HE3	1:B:368:PHE:CE1	1.94	1.02
1:A:608:ARG:HG3	1:A:889:TRP:CZ3	1.96	0.99
1:A:773:THR:HG23	1:A:788:ALA:HB3	1.45	0.98
1:B:895:THR:HG22	5:B:2306:HOH:O	1.63	0.97
1:B:201:TRP:HE1	1:B:212:ASN:HD21	1.07	0.93
1:A:201:TRP:HE1	1:A:212:ASN:HD21	1.06	0.90
1:B:608:ARG:HG3	1:B:889:TRP:CZ3	2.11	0.84
1:A:577:ARG:HD2	1:A:652:HIS:ND1	1.93	0.83
1:A:577:ARG:HG2	1:A:583:PHE:O	1.80	0.81
1:A:424:GLU:O	1:A:428:ASN:HB2	1.80	0.80
1:B:577:ARG:HG2	1:B:583:PHE:O	1.83	0.79
1:B:109:MET:HE1	1:B:368:PHE:HE1	1.46	0.78
1:B:109:MET:HE2	1:B:368:PHE:CE1	2.19	0.76
1:B:846:LYS:HE3	1:B:847:PRO:HD2	1.70	0.72
1:B:336:ASP:H	1:B:352:ASN:ND2	1.89	0.71
1:B:109:MET:HE3	1:B:368:PHE:CZ	2.26	0.69
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.88	0.68
1:B:246:ASP:HB3	1:B:292:LEU:HD11	1.75	0.68
1:B:846:LYS:HE2	5:B:2207:HOH:O	1.94	0.68
1:B:94:LEU:O	1:B:99:LYS:HB2	1.95	0.67
1:A:685:ARG:NH1	1:A:736:VAL:O	2.30	0.65
1:A:201:TRP:HE1	1:A:212:ASN:ND2	1.88	0.65
1:A:336:ASP:H	1:A:352:ASN:ND2	1.94	0.65
1:A:659:TYR:O	1:A:660:MET:HB2	1.96	0.64
1:B:804:GLY:HA3	1:B:824:LYS:O	1.97	0.64
1:B:109:MET:CE	1:B:368:PHE:CZ	2.80	0.63
1:A:364:THR:HG21	1:A:647:PRO:HD3	1.81	0.63
1:B:398:GLU:O	1:B:454:ARG:NH2	2.33	0.61
1:A:349:TYR:OH	1:A:494:ILE:HD11	2.01	0.60
1:A:704:THR:CG2	5:A:2247:HOH:O	2.51	0.59
1:A:577:ARG:HD2	1:A:652:HIS:CG	2.37	0.58
1:B:577:ARG:HD2	1:B:652:HIS:ND1	2.19	0.57
1:B:577:ARG:HD2	1:B:652:HIS:CG	2.41	0.56
1:B:311:ARG:HD3	5:B:2138:HOH:O	2.06	0.56
1:A:804:GLY:HA3	1:A:824:LYS:O	2.06	0.56
1:A:577:ARG:CG	1:A:583:PHE:O	2.53	0.56
1:B:335:ARG:HD3	1:B:459:PRO:O	2.04	0.56
1:B:753:THR:HG23	5:B:2274:HOH:O	2.06	0.56
1:A:211:GLN:HG3	5:A:2055:HOH:O	2.04	0.56
1:A:773:THR:CG2	1:A:788:ALA:HB3	2.30	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:THR:OG1	1:A:787:SER:OG	2.25	0.55
1:A:311:ARG:CD	5:A:2092:HOH:O	2.55	0.54
1:A:337:VAL:HG13	1:A:491:LEU:CD2	2.36	0.54
1:B:659:TYR:O	1:B:660:MET:HB2	2.07	0.54
1:A:677:HIS:CD2	1:A:679:GLN:HE21	2.26	0.54
1:B:72:SER:O	1:B:183:SER:HB2	2.08	0.53
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.72	0.53
1:A:677:HIS:HD2	1:A:679:GLN:HE21	1.58	0.52
1:B:191:ASN:O	1:B:211:GLN:HG2	2.09	0.52
1:B:808:ASN:HD22	1:B:809:SER:H	1.57	0.52
1:B:885:ARG:HD3	5:B:2302:HOH:O	2.09	0.52
1:B:804:GLY:O	1:B:823:LEU:HA	2.10	0.51
1:A:398:GLU:O	1:A:454:ARG:NH2	2.41	0.51
1:A:311:ARG:HD3	5:A:2092:HOH:O	2.09	0.51
1:A:441:TYR:HB2	1:A:442:PRO:HD3	1.93	0.51
1:A:202:ILE:HG22	1:A:203:ASP:H	1.74	0.50
1:B:704:THR:CG2	5:B:2262:HOH:O	2.59	0.50
1:A:465:HIS:HD2	5:A:2155:HOH:O	1.93	0.50
1:B:577:ARG:CG	1:B:583:PHE:O	2.57	0.49
1:A:94:LEU:HD22	1:A:99:LYS:HD2	1.94	0.49
1:A:202:ILE:HG22	1:A:203:ASP:N	2.28	0.49
1:A:608:ARG:HG2	1:A:609:LYS:N	2.28	0.49
1:B:144:LEU:HD22	1:B:165:ALA:CB	2.43	0.48
1:A:676:LEU:HD23	1:A:760:VAL:HG21	1.95	0.48
1:A:106:SER:OG	1:A:562:GLU:OE2	2.32	0.48
1:A:700:LEU:HD23	1:A:754:ASP:HA	1.95	0.48
1:B:452:ALA:HB1	1:B:489:PHE:HB2	1.96	0.48
1:B:671:LYS:O	1:B:677:HIS:CE1	2.68	0.47
1:A:874:THR:O	1:A:877:LEU:HB2	2.15	0.47
1:B:465:HIS:HD2	5:B:2170:HOH:O	1.97	0.47
1:A:72:SER:O	1:A:183:SER:HB2	2.15	0.47
1:B:609:LYS:CE	1:B:796:ASN:HD21	2.28	0.47
1:B:311:ARG:CD	5:B:2138:HOH:O	2.61	0.47
1:B:895:THR:HG21	5:B:2121:HOH:O	2.14	0.46
1:B:661:ASP:OD1	1:B:839:LYS:NZ	2.48	0.46
1:B:744:THR:O	1:B:768:SER:HA	2.16	0.46
1:A:577:ARG:HD3	1:A:652:HIS:HB3	1.97	0.46
1:B:357:LEU:HD23	1:B:359:ARG:HD3	1.97	0.46
1:A:704:THR:HG23	5:A:2247:HOH:O	2.12	0.46
1:A:411:VAL:O	1:A:460:SER:HB2	2.15	0.46
1:A:50:ASN:ND2	1:A:52:THR:OG1	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.99	0.45
1:A:608:ARG:HG3	1:A:889:TRP:HZ3	1.70	0.45
1:A:701:THR:HB	1:A:720:THR:HA	1.98	0.45
1:A:139:ASP:OD2	1:A:222:ARG:NH1	2.49	0.45
1:B:144:LEU:HA	1:B:145:SER:HA	1.80	0.45
1:B:411:VAL:O	1:B:460:SER:HB2	2.16	0.44
1:B:538:PHE:CD1	1:B:638:GLY:HA3	2.52	0.44
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.82	0.44
1:A:377:ALA:HA	1:A:405:ILE:HG21	1.98	0.44
1:B:109:MET:HE2	1:B:368:PHE:CZ	2.52	0.44
1:A:418:GLU:OE2	1:A:421:ASP:OD2	2.36	0.44
1:B:803:VAL:O	1:B:894:GLN:NE2	2.51	0.44
1:B:605:ASP:OD1	1:B:608:ARG:HD3	2.18	0.43
1:B:311:ARG:HD2	1:B:407:ASP:HB3	2.00	0.43
1:A:131:ASP:OD2	1:A:133:SER:HB2	2.18	0.43
1:A:155:LYS:HD3	1:A:158:THR:HG22	2.00	0.43
1:A:515:PRO:HD2	1:A:542:THR:OG1	2.19	0.43
1:A:143:VAL:HG23	1:A:143:VAL:O	2.17	0.43
1:A:659:TYR:O	1:A:660:MET:CB	2.62	0.43
1:A:468:SER:O	1:A:497:ALA:N	2.45	0.43
1:B:537:SER:OG	1:B:538:PHE:N	2.50	0.43
1:B:433:GLY:N	5:B:2153:HOH:O	2.51	0.43
1:A:609:LYS:NZ	1:A:796:ASN:HD21	2.17	0.43
1:B:700:LEU:HD23	1:B:754:ASP:HA	2.01	0.43
1:B:311:ARG:NH2	1:B:404:ASP:OD1	2.49	0.42
1:A:144:LEU:HD22	1:A:165:ALA:CB	2.48	0.42
1:B:159:LYS:HD3	1:B:189:TYR:CZ	2.54	0.42
1:A:566:MET:HG3	1:A:586:LEU:HD11	2.01	0.42
1:A:193:PRO:HD3	1:A:211:GLN:HG2	1.99	0.42
1:B:874:THR:O	1:B:877:LEU:HB2	2.19	0.42
1:B:805:ALA:CB	1:B:886:ILE:HD13	2.49	0.42
1:B:609:LYS:HE3	1:B:796:ASN:HD21	1.84	0.42
1:A:349:TYR:OH	1:A:494:ILE:CD1	2.66	0.42
1:A:137:TYR:HB2	1:A:222:ARG:HB2	2.00	0.42
1:A:230:ARG:HG2	5:A:2039:HOH:O	2.19	0.42
1:A:682:HIS:HE1	5:A:2207:HOH:O	2.01	0.42
1:B:605:ASP:HA	1:B:608:ARG:HD3	2.01	0.42
1:A:578:SER:HB3	1:A:583:PHE:O	2.20	0.42
1:A:569:ASN:OD1	1:A:571:SER:HB2	2.20	0.42
1:B:463:SER:HB2	1:B:494:ILE:HD12	2.02	0.41
1:A:246:ASP:HB3	1:A:292:LEU:HD11	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:HE1	1:B:208:PRO:HA	2.01	0.41
1:A:744:THR:O	1:A:768:SER:HA	2.20	0.41
1:B:642:TRP:HA	1:B:643:MET:HA	1.82	0.41
1:B:805:ALA:HB2	1:B:886:ILE:HD13	2.03	0.41
1:B:377:ALA:HA	1:B:405:ILE:HG21	2.03	0.41
1:B:605:ASP:HA	1:B:608:ARG:CD	2.51	0.41
1:B:682:HIS:HE1	5:B:2228:HOH:O	2.03	0.41
1:A:526:ASP:O	1:A:534:GLY:HA3	2.20	0.41
1:A:255:ASN:O	1:A:283:LYS:HA	2.21	0.41
1:A:787:SER:HA	5:A:2262:HOH:O	2.19	0.40
1:B:685:ARG:NH1	1:B:736:VAL:O	2.51	0.40
1:B:821:VAL:HG22	1:B:868:LEU:HB2	2.04	0.40
1:A:527:LYS:HE3	1:A:536:TRP:HB3	2.04	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)
5:A:2044:HOH:O	5:B:2099:HOH:O[1_655]	2.15	0.05

## 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	849/1032 (82%)	823 (97%)	22 (3%)	4 (0%)	34	34
1	B	845/1032 (82%)	824 (98%)	18 (2%)	3 (0%)	39	42
All	All	1694/2064 (82%)	1647 (97%)	40 (2%)	7 (0%)	39	42

All (7) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	469	GLU
1	A	597	TYR
1	B	469	GLU
1	B	597	TYR
1	A	431	GLU
1	B	202	ILE
1	A	202	ILE

### 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	698/834 (84%)	671 (96%)	27 (4%)	39	45
1	B	695/834 (83%)	671 (96%)	24 (4%)	43	51
All	All	1393/1668 (84%)	1342 (96%)	51 (4%)	41	48

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	144	LEU
1	A	211	GLN
1	A	230	ARG
1	A	237	LYS
1	A	335	ARG
1	A	337	VAL
1	A	356	LEU
1	A	430	GLU
1	A	469	GLU
1	A	561	SER
1	A	577	ARG
1	A	580	SER
1	A	586	LEU
1	A	608	ARG
1	A	648	TRP
1	A	652	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	698	SER
1	A	701	THR
1	A	704	THR
1	A	740	SER
1	A	773	THR
1	A	783	TYR
1	A	806	THR
1	A	846	LYS
1	A	877	LEU
1	A	895	THR
1	B	99	LYS
1	B	143	VAL
1	B	144	LEU
1	B	211	GLN
1	B	247	LEU
1	B	299	ASN
1	B	337	VAL
1	B	356	LEU
1	B	577	ARG
1	B	597	TYR
1	B	608	ARG
1	B	648	TRP
1	B	652	HIS
1	B	701	THR
1	B	704	THR
1	B	724	VAL
1	B	780	ASP
1	B	808	ASN
1	B	821	VAL
1	B	827	SER
1	B	830	ARG
1	B	846	LYS
1	B	877	LEU
1	B	895	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	A	352	ASN
1	A	465	HIS
1	A	529	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	679	GLN
1	A	682	HIS
1	A	750	ASN
1	A	786	GLN
1	A	796	ASN
1	A	808	ASN
1	B	116	GLN
1	B	128	ASN
1	B	176	GLN
1	B	194	ASN
1	B	212	ASN
1	B	299	ASN
1	B	352	ASN
1	B	465	HIS
1	B	682	HIS
1	B	750	ASN
1	B	796	ASN
1	B	808	ASN
1	B	894	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 18 ligands modelled in this entry, 13 are monoatomic - leaving 5 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	$\# Z  > 2$
3	ACT	A	1906	-	1,3,3	3.56	1 (100%)	0,3,3	0.00	-
4	GOL	A	1907	-	5,5,5	0.31	0	5,5,5	1.09	0
4	GOL	A	1908	-	5,5,5	0.39	0	5,5,5	0.55	0
3	ACT	B	1906	-	1,3,3	4.59	1 (100%)	0,3,3	0.00	-
4	GOL	B	1907	-	5,5,5	0.42	0	5,5,5	1.36	1 (20%)

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
3	ACT	A	1906	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1907	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1908	-	-	0/4/4/4	0/0/0/0
3	ACT	B	1906	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1907	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1906	ACT	CH3-C	3.56	1.53	1.48
3	B	1906	ACT	CH3-C	4.59	1.55	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1907	GOL	O2-C2-C3	2.30	119.19	108.65

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	851/1032 (82%)	-0.13	15 (1%)	71 73	17, 25, 35, 52	2 (0%)
1	B	849/1032 (82%)	-0.13	10 (1%)	81 82	16, 25, 35, 51	0
All	All	1700/2064 (82%)	-0.13	25 (1%)	76 78	16, 25, 35, 52	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	PRO	3.1
1	B	178	HIS	2.9
1	A	321	GLY	2.8
1	A	128	ASN	2.7
1	A	618	VAL	2.7
1	A	131	ASP	2.5
1	A	181	VAL	2.5
1	B	655	LEU	2.4
1	A	632	SER	2.4
1	B	279	SER	2.3
1	A	391	VAL	2.3
1	A	431	GLU	2.3
1	B	632	SER	2.2
1	A	843	SER	2.2
1	A	258	ALA	2.2
1	A	641	TYR	2.2
1	A	655	LEU	2.2
1	B	128	ASN	2.1
1	B	262	GLN	2.1
1	A	874	THR	2.1
1	B	323	THR	2.1
1	B	393	LEU	2.1
1	B	828	GLY	2.1
1	B	429	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	640	ILE	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
3	ACT	A	1906	4/4	0.63	0.30	5.45	32,32,33,33	0
3	ACT	B	1906	4/4	0.72	0.23	3.62	24,25,26,27	0
4	GOL	A	1907	6/6	0.86	0.24	3.37	36,39,40,41	0
4	GOL	B	1907	6/6	0.72	0.26	3.23	38,39,40,41	0
2	CD	B	1901	1/1	1.00	0.10	-0.17	25,25,25,25	0
2	CD	B	1900	1/1	0.99	0.08	-0.71	25,25,25,25	0
2	CD	A	1901	1/1	0.99	0.10	-1.39	37,37,37,37	0
2	CD	B	1903	1/1	0.99	0.10	-1.53	34,34,34,34	0
2	CD	B	1905	1/1	0.94	0.09	-	102,102,102,102	0
2	CD	A	1909	1/1	1.00	0.09	-	28,28,28,28	0
2	CD	A	1900	1/1	0.96	0.09	-	47,47,47,47	0
2	CD	A	1902	1/1	0.96	0.09	-	53,53,53,53	0
2	CD	B	1902	1/1	0.98	0.07	-	48,48,48,48	0
4	GOL	A	1908	6/6	0.91	0.14	-	39,43,46,47	0
2	CD	A	1904	1/1	0.93	0.09	-	105,105,105,105	0
2	CD	B	1904	1/1	0.89	0.06	-	100,100,100,100	0
2	CD	A	1903	1/1	0.18	0.90	-	295,295,295,295	0
2	CD	A	1905	1/1	0.97	0.05	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.