Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:27 AM BST

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*
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 ①) were used in the production of this report:

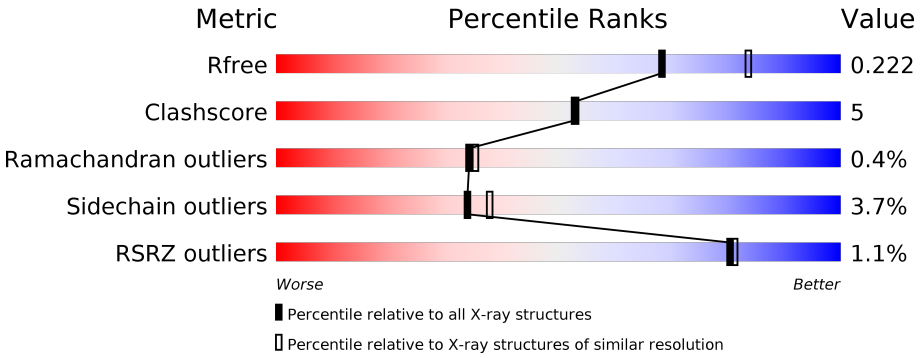
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 71% 9% • 18%
1	B	1032	72% 8% • 18%

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
2	CD	A	1903	-	-	-	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			

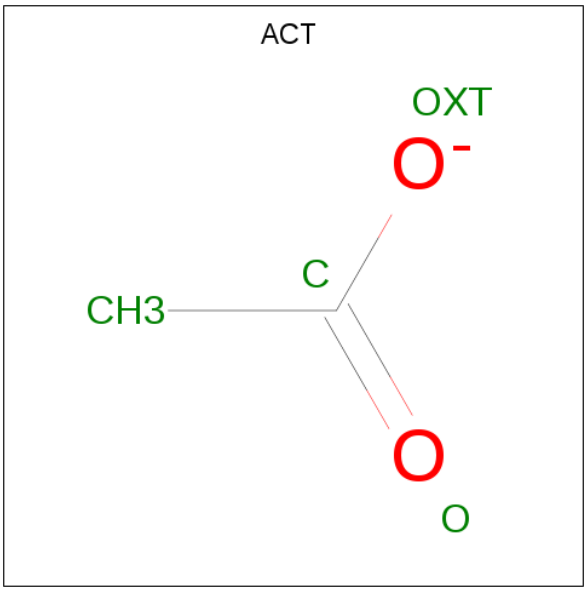
There are 4 discrepancies between the modelled and reference sequences:

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).

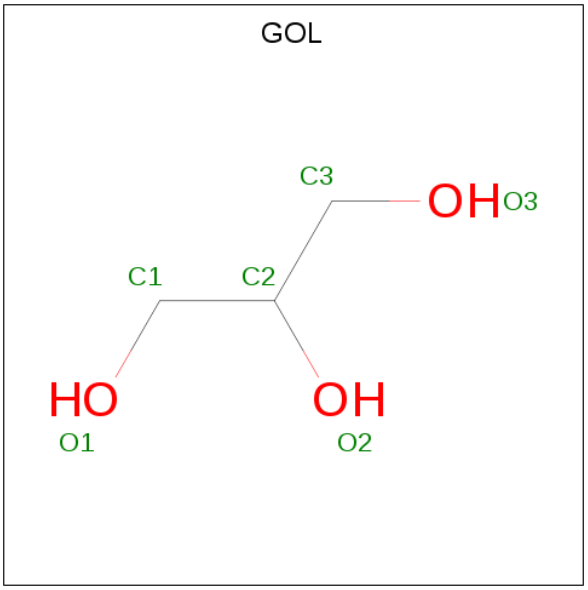
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Cd	0	0
			6	6		
2	A	7	Total	Cd	0	0
			7	7		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- 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 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

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

- Molecule 5 is water.

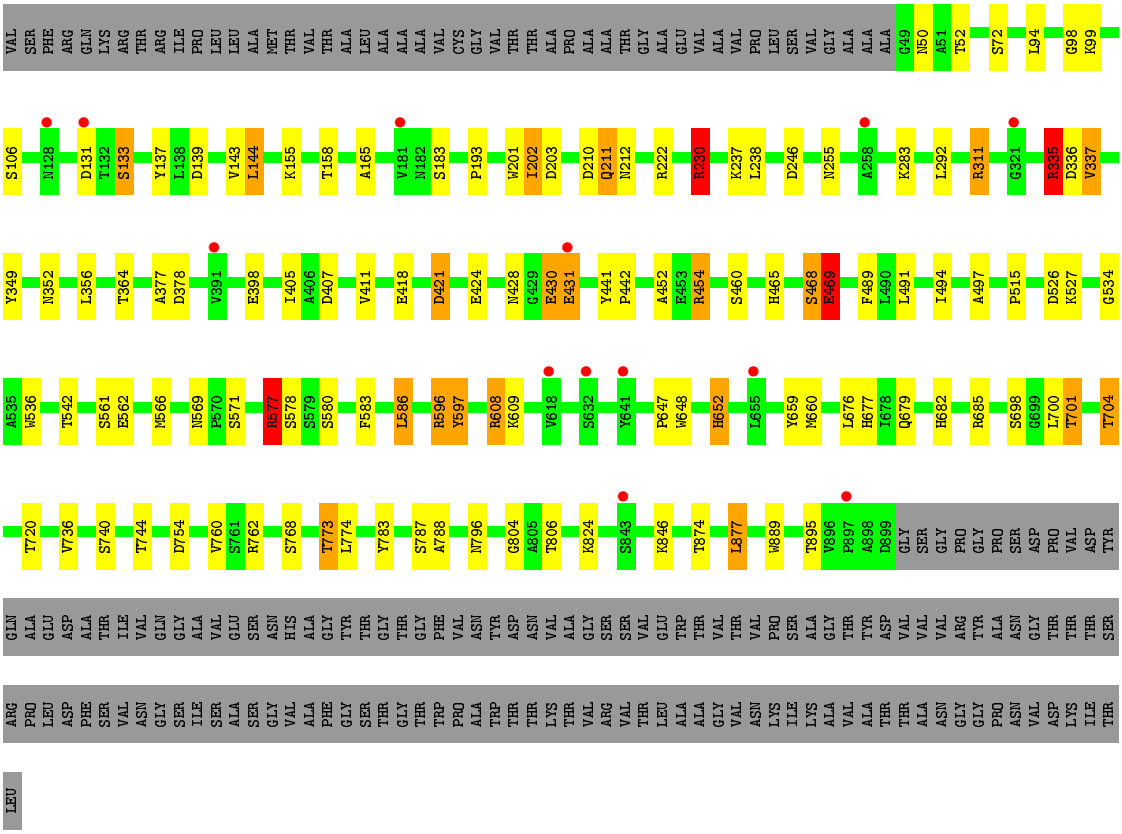
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	301	Total	O	0	0
			301	301		
5	B	306	Total	O	0	0
			306	306		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

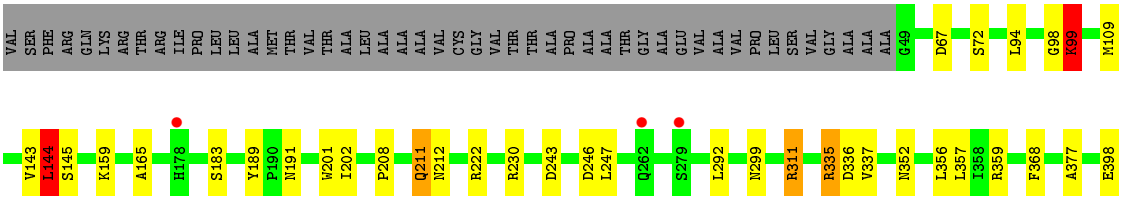
- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

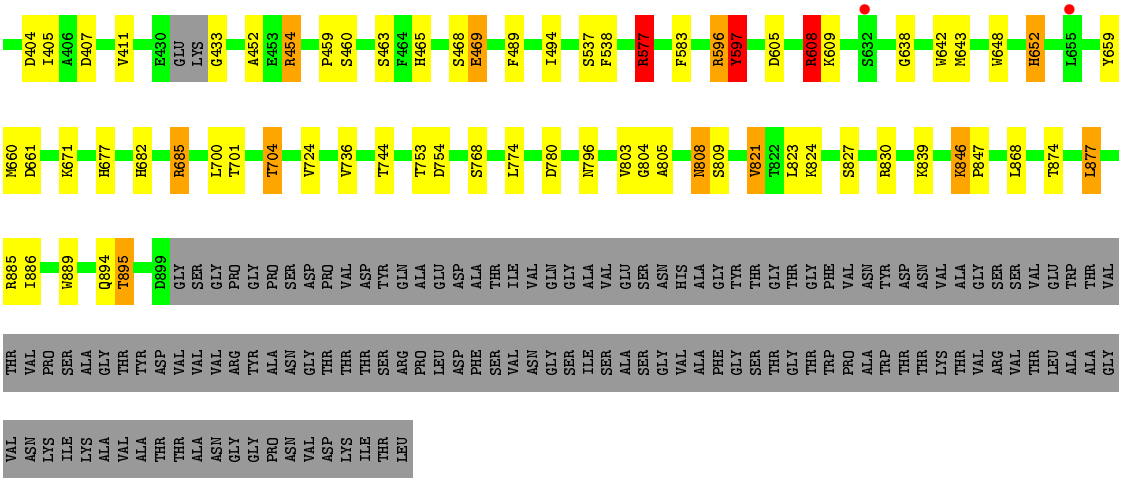
Chain A:



- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain B:




D404 I405 A406 D407 V411 E430 GLU LYS G433 A452 E453 R454 P459 S460 S463 F464 H465 S468 E469 F489 I494 S537 F538 R577 F583 R596 Y597 D605 R608 K609 S632 G638 W642 M643 W648 H652 L655 Y659
M660 D661 K671 H677 H682 R685 L700 T701 T704 V724 V736 T744 T753 D754 S768 L774 D780 N796 V803 G804 A805 N808 S809 V821 T822 L823 K824 S827 R830 K839 K846 P847 L868 T874 L877
R885 I886 W889 Q894 T895 D899 GLY SER GLY PRO GLY PRO SER ASP PRO VAL ASP TYR GLN ALA GLU ASP ALA THR ILE VAL GLN GLY ALA VAL GLU SER ASN HIS ALA GLY TYR THR GLY THR GLY PHE VAL ASN TYR ASP ASN VAL ALA GLY SER SER VAL GLU TRP THR VAL
THR VAL PRO SER ALA GLY THR TYR ASP VAL VAL VAL ARG TYR ALA ASN GLY THR THR THR SER ARG PRO LEU ASP PHE SER VAL ASN GLY SER ILE SER ALA SER GLY VAL ALA PHE GLY SER THR GLY THR TRP PRO ALA TRP THR THR LYS THR VAL ARG VAL THR LEU ALA ALA GLY
VAL ASN LYS ILE LYS ALA VAL ALA THR THR ALA ASN GLY GLY PRO ASN VAL ASP LYS ILE THR LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.40Å 122.03Å 91.60Å 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
$< I/\sigma(I) >$ [1]	5.24 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.223 0.175 , 0.222	Depositor DCC
R_{free} test set	4531 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13644	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (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	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

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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:A:804:GLY:HA3	1:A:824:LYS:O	2.06	0.56
1:B:311:ARG:HD3	5:B:2138:HOH:O	2.06	0.56
1:B:577:ARG:HD2	1:B:652:HIS:CG	2.41	0.56
1:A:211:GLN:HG3	5:A:2055:HOH:O	2.04	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:773:THR:CG2	1:A:788:ALA:HB3	2.30	0.55

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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:A:677:HIS:CD2	1:A:679:GLN:HE21	2.26	0.54
1:B:659:TYR:O	1:B:660:MET:HB2	2.07	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:A:398:GLU:O	1:A:454:ARG:NH2	2.41	0.51
1:B:804:GLY:O	1:B:823:LEU:HA	2.10	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:A:465:HIS:HD2	5:A:2155:HOH:O	1.93	0.50
1:B:704:THR:CG2	5:B:2262:HOH:O	2.59	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:661:ASP:OD1	1:B:839:LYS:NZ	2.48	0.46
1:B:895:THR:HG21	5:B:2121:HOH:O	2.14	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:411:VAL:O	1:A:460:SER:HB2	2.15	0.46
1:A:704:THR:HG23	5:A:2247:HOH:O	2.12	0.46
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASN:ND2	1:A:52:THR:OG1	2.47	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:311:ARG:HD2	1:B:407:ASP:HB3	2.00	0.43
1:B:605:ASP:OD1	1:B:608:ARG:HD3	2.18	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:143:VAL:HG23	1:A:143:VAL:O	2.17	0.43
1:A:515:PRO:HD2	1:A:542:THR:OG1	2.19	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:433:GLY:N	5:B:2153:HOH:O	2.51	0.43
1:B:537:SER:OG	1:B:538:PHE:N	2.50	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:A:144:LEU:HD22	1:A:165:ALA:CB	2.48	0.42
1:A:566:MET:HG3	1:A:586:LEU:HD11	2.01	0.42
1:B:159:LYS:HD3	1:B:189:TYR:CZ	2.54	0.42
1:B:311:ARG:NH2	1:B:404:ASP:OD1	2.49	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:A:569:ASN:OD1	1:A:571:SER:HB2	2.20	0.42
1:A:578:SER:HB3	1:A:583:PHE:O	2.20	0.42
1:B:605:ASP:HA	1:B:608:ARG:HD3	2.01	0.42
1:A:246:ASP:HB3	1:A:292:LEU:HD11	2.02	0.41
1:B:463:SER:HB2	1:B:494:ILE:HD12	2.02	0.41

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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:255:ASN:O	1:A:283:LYS:HA	2.21	0.41
1:A:526:ASP:O	1:A:534:GLY:HA3	2.20	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%)	29	28
1	B	845/1032 (82%)	824 (98%)	18 (2%)	3 (0%)	34	35
All	All	1694/2064 (82%)	1647 (97%)	40 (2%)	7 (0%)	34	35

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 (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	698/834 (84%)	671 (96%)	27 (4%)	32	35
1	B	695/834 (83%)	671 (96%)	24 (4%)	36	40
All	All	1393/1668 (84%)	1342 (96%)	51 (4%)	34	38

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

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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

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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

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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	GOL	B	1907	-	5,5,5	0.48	0	5,5,5	1.34	1 (20%)
3	ACT	B	1906	-	1,3,3	5.05	1 (100%)	0,3,3	0.00	-
4	GOL	A	1908	-	5,5,5	0.41	0	5,5,5	0.54	0
3	ACT	A	1906	-	1,3,3	3.93	1 (100%)	0,3,3	0.00	-
4	GOL	A	1907	-	5,5,5	0.37	0	5,5,5	1.05	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
4	GOL	B	1907	-	-	3/4/4/4	-
4	GOL	A	1907	-	-	3/4/4/4	-
4	GOL	A	1908	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1906	ACT	CH3-C	5.05	1.55	1.48
3	A	1906	ACT	CH3-C	3.93	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1907	GOL	O2-C2-C3	2.29	119.19	109.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1907	GOL	O1-C1-C2-O2
4	A	1907	GOL	O1-C1-C2-C3
4	B	1907	GOL	O1-C1-C2-C3
4	A	1908	GOL	O1-C1-C2-O2
4	A	1907	GOL	C1-C2-C3-O3
4	A	1908	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	1907	GOL	C1-C2-C3-O3
4	B	1907	GOL	O1-C1-C2-O2
4	A	1908	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	A	851/1032 (82%)	-0.18	13 (1%) 73 74	17, 25, 35, 52	2 (0%)
1	B	849/1032 (82%)	-0.18	5 (0%) 89 89	16, 25, 35, 51	0
All	All	1700/2064 (82%)	-0.18	18 (1%) 80 81	16, 25, 35, 52	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	PRO	3.0
1	B	178	HIS	2.8
1	A	321	GLY	2.6
1	A	128	ASN	2.6
1	A	618	VAL	2.5
1	A	131	ASP	2.4
1	B	655	LEU	2.3
1	A	181	VAL	2.3
1	A	632	SER	2.3
1	B	279	SER	2.2
1	A	431	GLU	2.2
1	A	843	SER	2.1
1	A	258	ALA	2.1
1	A	391	VAL	2.1
1	B	632	SER	2.1
1	A	641	TYR	2.1
1	A	655	LEU	2.1
1	B	262	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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^2)	Q<0.9
2	CD	A	1903	1/1	0.18	0.90	295,295,295,295	0
3	ACT	A	1906	4/4	0.63	0.30	32,32,33,33	0
4	GOL	B	1907	6/6	0.72	0.26	38,39,40,41	0
3	ACT	B	1906	4/4	0.73	0.23	24,25,26,27	0
4	GOL	A	1907	6/6	0.86	0.24	36,39,40,41	0
2	CD	B	1904	1/1	0.90	0.06	100,100,100,100	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	1905	1/1	0.94	0.09	102,102,102,102	0
2	CD	A	1902	1/1	0.96	0.09	53,53,53,53	0
2	CD	A	1900	1/1	0.96	0.09	47,47,47,47	0
2	CD	A	1905	1/1	0.97	0.05	76,76,76,76	0
2	CD	B	1902	1/1	0.98	0.07	48,48,48,48	0
2	CD	B	1900	1/1	0.99	0.08	25,25,25,25	0
2	CD	A	1901	1/1	0.99	0.10	37,37,37,37	0
2	CD	B	1903	1/1	0.99	0.10	34,34,34,34	0
2	CD	B	1901	1/1	1.00	0.10	25,25,25,25	0
2	CD	A	1909	1/1	1.00	0.09	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.