Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:10 PM BST

PDB ID	:	2VZS
Title	:	Chitosan Product complex 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	:	1.85 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:

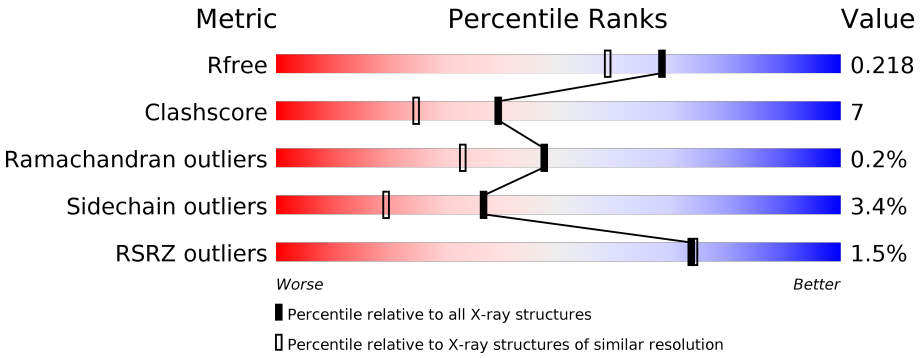
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	% 72% 9% • 17%
1	B	1032	% 73% 9% • 17%

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	1899	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14981 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	858	Total	C	N	O	S	4	0	1
			6552	4115	1133	1287	17			
1	B	858	Total	C	N	O	S	0	0	1
			6552	4115	1133	1287	17			

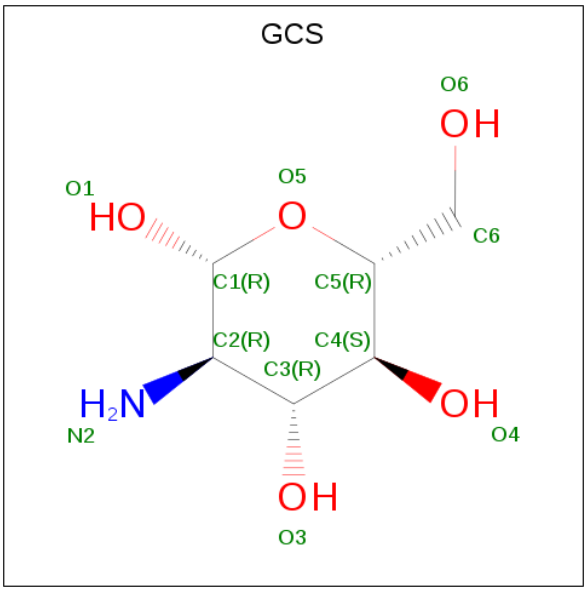
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	750	ASN	TRP	conflict	UNP Q56F26
B	750	ASN	TRP	conflict	UNP Q56F26

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

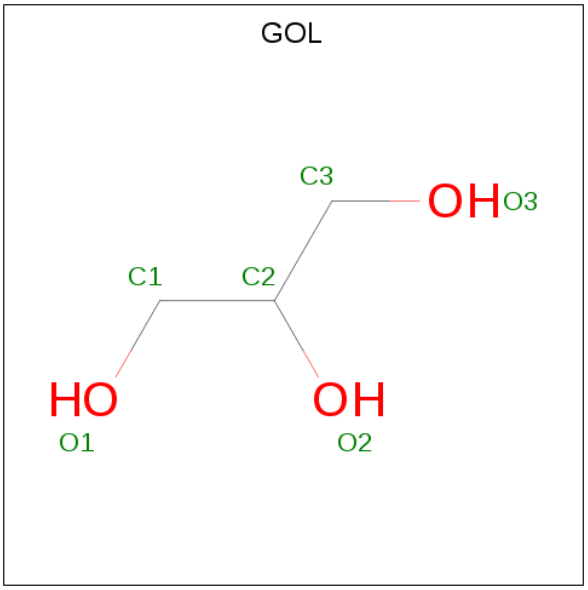
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cd	0	0
			3	3		
2	A	3	Total	Cd	0	0
			3	3		

- Molecule 3 is 2-amino-2-deoxy-beta-D-glucopyranose (three-letter code: GCS) (formula: $C_6H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	1	5		
3	B	1	Total	C	N	O	0	0
			12	6	1	5		

- 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	B	1	Total	C	O		0	0
			6	3	3			

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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.

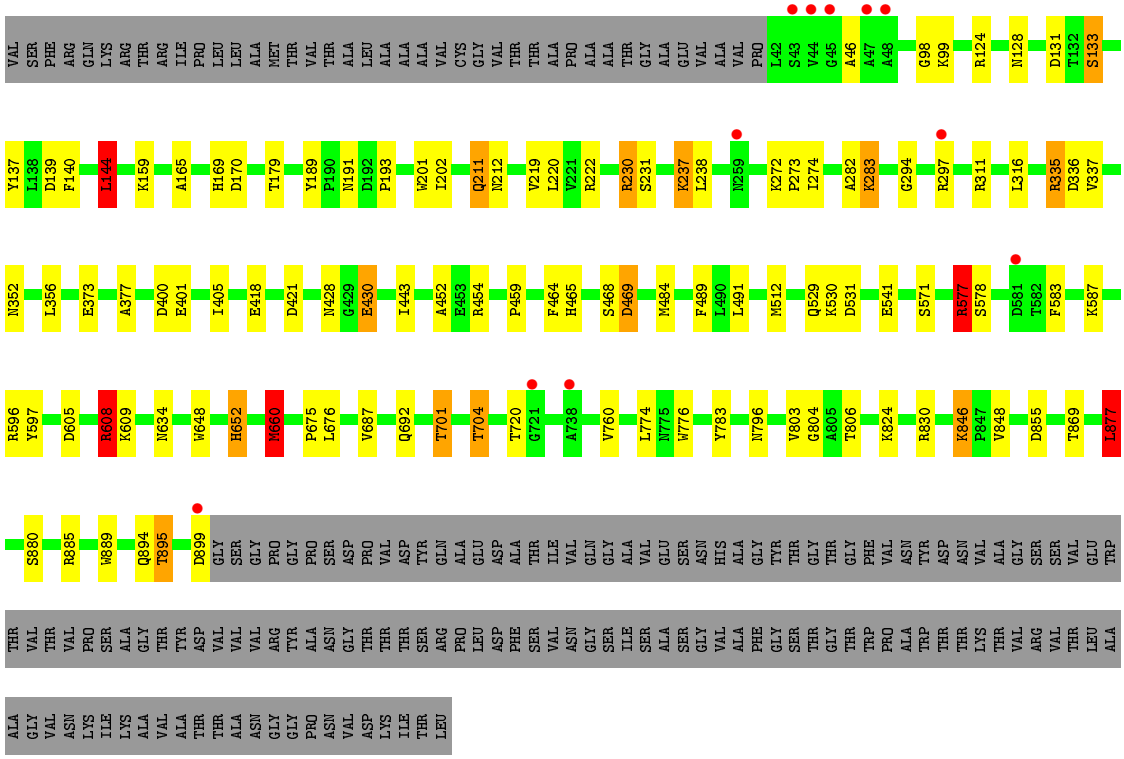
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	958	Total	O	0	0
			958	958		
5	B	871	Total	O	0	0
			871	871		

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.

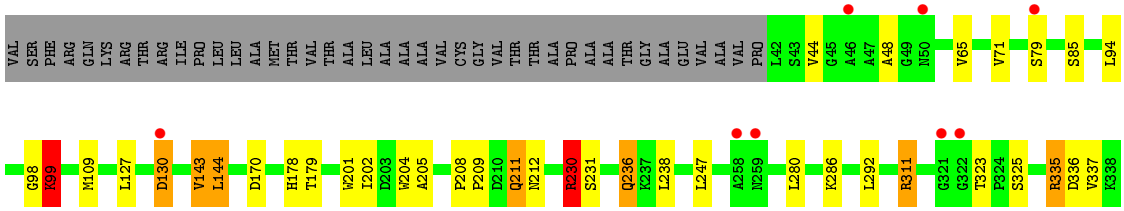
- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

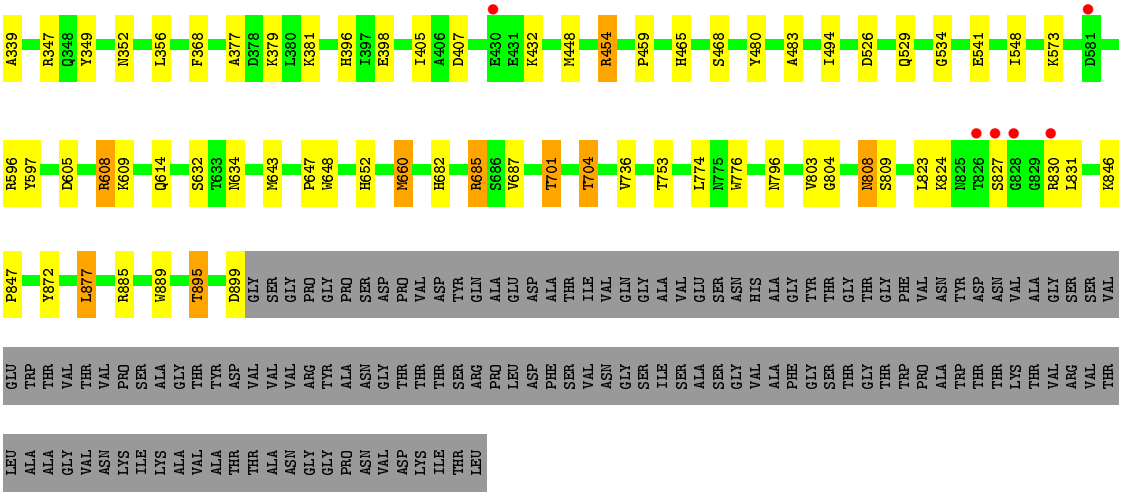
Chain A:



- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain B:




A339 R347 Q348 Y349 N352 L356 F368 A377 D378 K379 L380 K381 H396 I397 E398 I405 A406 D407 E430 E431 K432 M448 R454 P459 H465 S468 Y480 A483 I494 D526 Q529 G534 E541 I548 K573 D581
R596 V597 D605 R608 K609 Q614 S632 T633 N634 M643 P647 W648 H652 M660 H662 R685 S686 V687 T701 T704 V736 T753 L774 N775 W776 N796 V803 G804 N808 S809 L823 K824 N825 T826 S827 G828 G829 R830 L831 K846
P847 Y872 L877 R885 W889 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 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	86.54Å 121.81Å 91.84Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.85) 99.9 (19.99-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.220 0.172 , 0.218	Depositor DCC
R_{free} test set	8098 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14981	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, GCS, CD

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	0.90	1/6715 (0.0%)	0.97	23/9163 (0.3%)
1	B	0.90	2/6715 (0.0%)	1.04	25/9163 (0.3%)
All	All	0.90	3/13430 (0.0%)	1.00	48/18326 (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	0	3
1	B	0	3
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	12.05	1.75	1.52
1	B	335	ARG	CD-NE	-6.21	1.35	1.46
1	B	454	ARG	CD-NE	-5.79	1.36	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	335	ARG	NE-CZ-NH2	-28.58	106.01	120.30
1	B	454	ARG	NE-CZ-NH2	-27.75	106.43	120.30
1	A	335	ARG	NE-CZ-NH2	-26.63	106.99	120.30
1	A	335	ARG	NE-CZ-NH1	21.46	131.03	120.30
1	B	454	ARG	NE-CZ-NH1	21.35	130.98	120.30
1	B	335	ARG	NE-CZ-NH1	19.61	130.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	577	ARG	NE-CZ-NH1	17.89	129.24	120.30
1	A	230	ARG	NE-CZ-NH2	-13.73	113.43	120.30
1	A	577	ARG	NE-CZ-NH2	-13.51	113.54	120.30
1	B	311	ARG	NE-CZ-NH2	-12.97	113.81	120.30
1	A	230	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	B	230	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	B	311	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	A	660	MET	CG-SD-CE	-9.42	85.13	100.20
1	A	335	ARG	CD-NE-CZ	8.87	136.01	123.60
1	A	238	LEU	CA-CB-CG	8.81	135.56	115.30
1	B	454	ARG	CD-NE-CZ	8.58	135.61	123.60
1	B	335	ARG	CD-NE-CZ	8.46	135.44	123.60
1	B	597	TYR	N-CA-C	8.00	132.60	111.00
1	B	335	ARG	CG-CD-NE	-7.99	95.02	111.80
1	A	608	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	774	LEU	CA-CB-CG	-7.55	97.94	115.30
1	B	454	ARG	CG-CD-NE	-7.44	96.18	111.80
1	A	597	TYR	N-CA-C	7.40	130.99	111.00
1	A	577	ARG	CD-NE-CZ	7.25	133.75	123.60
1	B	144	LEU	CA-CB-CG	7.20	131.87	115.30
1	B	660	MET	CG-SD-CE	-7.20	88.67	100.20
1	A	774	LEU	CA-CB-CG	-7.15	98.86	115.30
1	A	335	ARG	CG-CD-NE	-7.10	96.89	111.80
1	B	230	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	144	LEU	CA-CB-CG	6.49	130.22	115.30
1	B	685	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	236	GLN	CA-CB-CG	6.40	127.48	113.40
1	A	885	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	608	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	855	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	877	LEU	CB-CG-CD1	5.62	120.56	111.00
1	B	238	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	130	ASP	CB-CA-C	-5.57	99.26	110.40
1	A	124	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	99	LYS	N-CA-C	-5.37	96.50	111.00
1	A	430	GLU	CB-CG-CD	5.30	128.51	114.20
1	B	127	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	99	LYS	N-CA-C	-5.14	97.12	111.00
1	B	143	VAL	CG1-CB-CG2	5.05	118.98	110.90
1	A	877	LEU	CA-CB-CG	5.03	126.87	115.30
1	B	292	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	A	877	LEU	CB-CG-CD1	5.01	119.51	111.00

There are no chirality outliers.

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	6552	0	6328	100	0
1	B	6552	0	6328	92	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	12	0	13	1	0
3	B	12	0	13	1	0
4	A	6	0	8	0	0
4	B	12	0	15	0	0
5	A	958	0	0	40	1
5	B	871	0	0	45	1
All	All	14981	0	12705	192	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 7.

All (192) 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:643:MET:CE	5:B:2625:HOH:O	1.81	1.26
1:B:483:ALA:HB3	5:B:2492:HOH:O	1.30	1.24
1:A:512:MET:HE1	5:A:2516:HOH:O	1.39	1.18
1:B:753:THR:HB	5:B:2719:HOH:O	1.39	1.18
1:A:846:LYS:HG2	5:A:2389:HOH:O	1.41	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:CE	1:B:209:PRO:HD3	1.78	1.12
1:B:109:MET:HE1	1:B:368:PHE:HE1	1.07	1.10
1:A:660:MET:SD	5:A:2434:HOH:O	2.07	1.10
1:B:204:TRP:HE3	5:B:2375:HOH:O	1.37	1.07
1:B:109:MET:HE2	1:B:209:PRO:CD	1.84	1.06
1:B:647:PRO:HG3	5:B:2375:HOH:O	1.55	1.05
1:B:643:MET:HE3	5:B:2625:HOH:O	1.42	1.04
1:A:401:GLU:HB3	5:A:2429:HOH:O	1.58	1.03
1:B:109:MET:CE	1:B:368:PHE:HE1	1.70	1.03
1:A:577:ARG:HD2	1:A:652:HIS:ND1	1.74	1.01
1:A:541:GLU:HG3	5:A:2596:HOH:O	1.64	0.98
1:A:660:MET:CE	5:A:2434:HOH:O	2.12	0.97
1:B:109:MET:HE1	1:B:368:PHE:CE1	1.99	0.97
1:B:109:MET:CE	1:B:368:PHE:CE1	2.48	0.96
1:B:201:TRP:HE1	1:B:212:ASN:HD21	1.07	0.96
1:A:512:MET:CE	5:A:2516:HOH:O	2.01	0.94
1:A:541:GLU:CG	5:A:2596:HOH:O	2.15	0.94
1:A:201:TRP:HE1	1:A:212:ASN:HD21	1.03	0.93
1:A:46:ALA:HB1	5:A:2094:HOH:O	1.69	0.91
1:A:846:LYS:CG	5:A:2389:HOH:O	2.09	0.89
1:B:846:LYS:HE3	5:B:2543:HOH:O	1.73	0.89
1:A:297:ARG:HG3	5:B:2018:HOH:O	1.72	0.89
1:A:634:ASN:HB3	5:A:2686:HOH:O	1.71	0.88
1:B:179:THR:CA	5:B:2183:HOH:O	2.21	0.88
1:A:297:ARG:HB2	5:A:2319:HOH:O	1.74	0.88
1:B:846:LYS:HE2	1:B:847:PRO:HD2	1.53	0.88
1:A:443:ILE:HD12	5:A:2492:HOH:O	1.73	0.87
1:A:179:THR:CA	5:A:2170:HOH:O	2.22	0.87
1:A:311:ARG:HD2	5:A:2511:HOH:O	1.74	0.87
1:B:480:TYR:HA	5:B:2492:HOH:O	1.77	0.85
1:B:605:ASP:HA	1:B:608:ARG:HD3	1.58	0.85
1:B:109:MET:HE2	1:B:209:PRO:HD3	0.90	0.84
1:B:895:THR:HG22	5:B:2860:HOH:O	1.77	0.83
1:B:541:GLU:OE2	3:B:1903:GCS:H1	1.79	0.81
1:B:872:TYR:HB2	5:B:2814:HOH:O	1.81	0.81
1:A:201:TRP:HE1	1:A:212:ASN:ND2	1.78	0.80
1:A:846:LYS:CD	5:A:2389:HOH:O	2.30	0.79
1:A:577:ARG:HG2	1:A:583:PHE:O	1.83	0.78
1:A:128:ASN:HB2	5:A:2088:HOH:O	1.83	0.78
1:B:349:TYR:OH	1:B:494:ILE:HD11	1.84	0.77
1:A:577:ARG:HD2	1:A:652:HIS:CG	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ARG:HG3	1:A:889:TRP:CZ3	2.20	0.77
1:B:109:MET:HE3	1:B:368:PHE:CE1	2.18	0.77
1:B:803:VAL:HB	5:B:2774:HOH:O	1.84	0.76
1:A:899:ASP:N	5:A:2954:HOH:O	2.18	0.76
1:A:220:LEU:CD1	1:A:222:ARG:HH12	1.98	0.75
1:B:311:ARG:CD	5:B:2334:HOH:O	2.34	0.75
1:B:643:MET:HE1	5:B:2625:HOH:O	1.58	0.74
1:A:846:LYS:HE2	5:A:2601:HOH:O	1.87	0.73
1:A:220:LEU:HD12	1:A:222:ARG:HH12	1.52	0.73
1:B:311:ARG:HD2	5:B:2334:HOH:O	1.88	0.71
1:A:531:ASP:HB2	5:A:2592:HOH:O	1.88	0.71
1:B:685:ARG:NH1	1:B:736:VAL:O	2.22	0.71
1:B:831:LEU:O	5:B:2798:HOH:O	2.09	0.70
1:B:109:MET:CE	1:B:208:PRO:HA	2.21	0.70
1:A:311:ARG:CD	5:A:2511:HOH:O	2.36	0.70
1:B:432:LYS:HG2	5:B:2442:HOH:O	1.92	0.70
1:A:530:LYS:HB3	5:A:2231:HOH:O	1.92	0.69
1:B:179:THR:CA	5:B:2182:HOH:O	2.40	0.68
1:A:237:LYS:HA	1:A:237:LYS:HE3	1.76	0.68
1:A:46:ALA:CB	5:A:2094:HOH:O	2.33	0.66
1:B:109:MET:HE2	1:B:208:PRO:HA	1.78	0.66
1:B:381:LYS:HD2	5:B:2400:HOH:O	1.95	0.65
1:A:541:GLU:HG2	5:A:2596:HOH:O	1.91	0.65
1:A:701:THR:HB	1:A:720:THR:HA	1.79	0.65
1:B:336:ASP:H	1:B:352:ASN:ND2	1.96	0.64
1:A:577:ARG:HD3	1:A:652:HIS:HB3	1.80	0.63
1:A:222:ARG:NE	5:A:2222:HOH:O	2.31	0.63
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.63	0.62
1:A:687:VAL:HG21	1:A:704:THR:HG21	1.80	0.62
1:A:541:GLU:OE2	3:A:1902:GCS:H1	2.01	0.60
1:A:336:ASP:H	1:A:352:ASN:ND2	1.98	0.60
1:A:634:ASN:CB	5:A:2686:HOH:O	2.37	0.59
1:B:94:LEU:O	1:B:99:LYS:HB2	2.03	0.59
1:B:335:ARG:HD3	1:B:459:PRO:O	2.03	0.59
1:A:131:ASP:OD2	1:A:133:SER:HB2	2.04	0.58
1:B:846:LYS:CE	5:B:2543:HOH:O	2.40	0.58
1:B:605:ASP:OD1	1:B:608:ARG:NH1	2.37	0.58
1:A:400:ASP:OD1	1:A:454:ARG:HD2	2.04	0.58
1:B:608:ARG:HG3	1:B:889:TRP:CZ3	2.39	0.57
1:A:220:LEU:HD12	1:A:222:ARG:NH1	2.19	0.57
1:B:895:THR:HG21	5:B:2862:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.89	0.56
1:B:204:TRP:CE3	5:B:2375:HOH:O	2.25	0.56
1:A:605:ASP:HA	1:A:608:ARG:HD3	1.87	0.56
1:B:48:ALA:HB1	1:B:325:SER:O	2.06	0.56
1:A:377:ALA:HA	1:A:405:ILE:HG21	1.88	0.56
1:B:701:THR:CG2	5:B:2667:HOH:O	2.55	0.55
1:A:170:ASP:OD2	1:A:230:ARG:HD2	2.07	0.55
1:A:804:GLY:HA3	1:A:824:LYS:O	2.06	0.55
1:B:529:GLN:HG3	1:B:776:TRP:CD2	2.42	0.55
1:A:335:ARG:HD3	1:A:459:PRO:O	2.07	0.54
1:A:605:ASP:HA	1:A:608:ARG:CD	2.38	0.54
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.72	0.54
1:B:448:MET:HG2	5:B:2492:HOH:O	2.07	0.54
1:B:548:ILE:H	1:B:614:GLN:NE2	2.05	0.54
1:A:830:ARG:HD2	5:A:2750:HOH:O	2.07	0.54
1:A:577:ARG:CD	1:A:652:HIS:CG	2.91	0.53
1:B:349:TYR:OH	1:B:494:ILE:CD1	2.54	0.53
1:B:899:ASP:N	5:B:2866:HOH:O	2.41	0.53
1:A:587:LYS:HE3	5:A:2646:HOH:O	2.07	0.53
1:B:573:LYS:HG3	5:B:2579:HOH:O	2.08	0.53
1:A:220:LEU:CD1	1:A:222:ARG:NH1	2.68	0.53
1:B:548:ILE:H	1:B:614:GLN:HE22	1.56	0.53
1:A:701:THR:CG2	5:A:2740:HOH:O	2.56	0.53
1:B:211:GLN:HG3	5:B:2228:HOH:O	2.08	0.53
1:B:609:LYS:CE	1:B:796:ASN:HD21	2.21	0.53
1:B:109:MET:HE1	1:B:208:PRO:HA	1.90	0.52
1:B:130:ASP:HB2	5:B:2001:HOH:O	2.09	0.52
1:A:191:ASN:O	1:A:211:GLN:HG2	2.10	0.52
1:B:704:THR:HG23	5:B:2668:HOH:O	2.10	0.51
1:B:701:THR:HG23	5:B:2667:HOH:O	2.11	0.51
1:A:220:LEU:HD13	1:A:222:ARG:HH12	1.75	0.51
1:B:647:PRO:CG	5:B:2375:HOH:O	2.32	0.50
1:A:608:ARG:HG2	1:A:609:LYS:N	2.26	0.50
1:A:701:THR:HG22	5:A:2740:HOH:O	2.11	0.50
1:B:311:ARG:HD3	5:B:2334:HOH:O	2.03	0.49
1:B:808:ASN:HD22	1:B:809:SER:H	1.61	0.49
1:B:687:VAL:HG21	1:B:704:THR:HG21	1.93	0.49
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.95	0.48
1:A:512:MET:HG3	5:A:2596:HOH:O	2.14	0.48
1:A:282:ALA:O	1:A:283:LYS:HB2	2.14	0.48
1:B:682:HIS:HE1	5:B:2611:HOH:O	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:895:THR:CG2	5:B:2860:HOH:O	2.46	0.48
1:A:660:MET:HE2	5:A:2434:HOH:O	1.90	0.48
1:B:804:GLY:HA3	1:B:824:LYS:O	2.13	0.48
1:B:529:GLN:HG3	1:B:776:TRP:CE3	2.49	0.47
1:A:587:LYS:NZ	5:A:2645:HOH:O	2.48	0.47
1:B:230:ARG:HG3	5:B:2245:HOH:O	2.15	0.47
1:B:65:VAL:HG11	1:B:71:VAL:CG2	2.45	0.47
1:B:753:THR:HG23	5:B:2718:HOH:O	2.14	0.47
1:A:443:ILE:CD1	5:A:2492:HOH:O	2.43	0.47
1:B:398:GLU:O	1:B:454:ARG:NH2	2.45	0.47
1:A:676:LEU:HD23	1:A:760:VAL:HG21	1.97	0.46
1:A:529:GLN:HG3	1:A:776:TRP:CE3	2.50	0.46
1:A:464:PHE:HB3	1:A:484:MET:HE1	1.97	0.46
1:A:571:SER:OG	1:A:587:LYS:HG3	2.16	0.46
1:A:139:ASP:OD2	1:A:222:ARG:NH1	2.49	0.46
1:A:159:LYS:HD3	1:A:189:TYR:CZ	2.51	0.45
1:B:377:ALA:HA	1:B:405:ILE:HG21	1.98	0.45
1:B:804:GLY:O	1:B:823:LEU:HA	2.15	0.45
1:A:144:LEU:HD22	1:A:165:ALA:CB	2.47	0.45
1:B:280:LEU:HD21	1:B:286:LYS:HB2	1.98	0.45
1:B:396:HIS:HB2	5:B:2374:HOH:O	2.15	0.45
1:B:379:LYS:HG2	1:B:660:MET:HE1	1.98	0.45
1:A:237:LYS:HE3	1:A:237:LYS:CA	2.44	0.45
1:A:609:LYS:CE	1:A:796:ASN:HD21	2.29	0.45
1:A:704:THR:HG23	5:A:2741:HOH:O	2.17	0.45
1:A:605:ASP:OD1	1:A:608:ARG:HD3	2.17	0.44
1:B:349:TYR:HH	1:B:494:ILE:HD11	1.83	0.44
1:B:336:ASP:H	1:B:352:ASN:HD22	1.63	0.44
1:A:609:LYS:NZ	1:A:796:ASN:HD21	2.16	0.43
1:A:220:LEU:HD13	1:A:222:ARG:NH1	2.33	0.43
1:A:373:GLU:HG3	5:A:2429:HOH:O	2.18	0.43
1:A:577:ARG:CD	1:A:652:HIS:HB3	2.48	0.43
1:B:846:LYS:HD2	5:B:2810:HOH:O	2.18	0.43
1:A:418:GLU:OE2	1:A:421:ASP:OD2	2.37	0.43
1:A:848:VAL:HG21	1:A:877:LEU:HD13	2.00	0.43
1:B:526:ASP:O	1:B:534:GLY:HA3	2.18	0.43
1:B:609:LYS:NZ	1:B:796:ASN:HD21	2.17	0.43
1:B:178:HIS:HD2	1:B:179:THR:O	2.01	0.43
1:B:339:ALA:HB1	1:B:347:ARG:HD2	2.01	0.43
1:A:336:ASP:H	1:A:352:ASN:HD22	1.65	0.43
1:A:803:VAL:O	1:A:894:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD11	1:A:316:LEU:HD21	2.00	0.43
1:A:577:ARG:HG3	1:A:578:SER:N	2.34	0.42
1:A:222:ARG:CZ	5:A:2222:HOH:O	2.65	0.42
1:A:895:THR:HG23	5:A:2951:HOH:O	2.19	0.42
1:B:170:ASP:OD2	1:B:230:ARG:HD3	2.20	0.42
1:A:140:PHE:HB3	1:A:219:VAL:HA	2.02	0.42
1:A:337:VAL:CG1	1:A:491:LEU:CD2	2.98	0.42
1:B:846:LYS:HE2	1:B:847:PRO:CD	2.35	0.42
1:B:465:HIS:HD2	5:B:2477:HOH:O	2.02	0.42
1:B:824:LYS:HG3	5:B:2828:HOH:O	2.19	0.42
1:A:139:ASP:HA	1:A:169:HIS:O	2.19	0.42
1:A:237:LYS:HE2	5:A:2376:HOH:O	2.20	0.42
1:A:193:PRO:O	1:A:421:ASP:HB2	2.19	0.41
1:B:704:THR:CG2	5:B:2668:HOH:O	2.66	0.41
1:B:827:SER:HB3	5:B:2798:HOH:O	2.19	0.41
1:B:885:ARG:HD3	5:B:2808:HOH:O	2.20	0.41
1:B:311:ARG:HD2	1:B:407:ASP:HB3	2.02	0.41
1:A:137:TYR:HB2	1:A:222:ARG:HB2	2.03	0.41
1:A:465:HIS:HD2	5:A:2514:HOH:O	2.04	0.40
1:A:877:LEU:HG	1:A:880:SER:O	2.21	0.40
1:A:272:LYS:HE3	1:A:294:GLY:O	2.22	0.40
1:A:273:PRO:HG3	5:B:2061:HOH:O	2.22	0.40
1:A:675:PRO:HA	1:A:692:GLN:HB2	2.03	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:2020:HOH:O	5:B:2658:HOH:O[1_655]	2.00	0.20

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	856/1032 (83%)	838 (98%)	16 (2%)	2 (0%)	47	33
1	B	856/1032 (83%)	833 (97%)	21 (2%)	2 (0%)	47	33
All	All	1712/2064 (83%)	1671 (98%)	37 (2%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	A	202	ILE
1	B	202	ILE
1	B	205	ALA

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	702/834 (84%)	679 (97%)	23 (3%)	38	21
1	B	702/834 (84%)	677 (96%)	25 (4%)	35	18
All	All	1404/1668 (84%)	1356 (97%)	48 (3%)	37	19

All (48) 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	231	SER
1	A	237	LYS
1	A	283	LYS
1	A	356	LEU
1	A	428	ASN
1	A	430	GLU
1	A	469	ASP
1	A	577	ARG
1	A	608	ARG

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Mol	Chain	Res	Type
1	A	648	TRP
1	A	652	HIS
1	A	660	MET
1	A	701	THR
1	A	704	THR
1	A	783	TYR
1	A	806	THR
1	A	846	LYS
1	A	869	THR
1	A	877	LEU
1	A	895	THR
1	B	44	VAL
1	B	79	SER
1	B	85	SER
1	B	99	LYS
1	B	143	VAL
1	B	144	LEU
1	B	211	GLN
1	B	230	ARG
1	B	231	SER
1	B	236	GLN
1	B	247	LEU
1	B	323	THR
1	B	337	VAL
1	B	356	LEU
1	B	608	ARG
1	B	632	SER
1	B	634	ASN
1	B	648	TRP
1	B	652	HIS
1	B	701	THR
1	B	704	THR
1	B	808	ASN
1	B	830	ARG
1	B	877	LEU
1	B	895	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	212	ASN

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Mol	Chain	Res	Type
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	679	GLN
1	A	682	HIS
1	A	750	ASN
1	A	796	ASN
1	A	808	ASN
1	B	50	ASN
1	B	128	ASN
1	B	176	GLN
1	B	178	HIS
1	B	194	ASN
1	B	212	ASN
1	B	299	ASN
1	B	348	GLN
1	B	352	ASN
1	B	465	HIS
1	B	614	GLN
1	B	682	HIS
1	B	796	ASN
1	B	808	ASN

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 11 ligands modelled in this entry, 6 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	GCS	A	1902	-	12,12,12	1.05	1 (8%)	16,17,17	1.98	4 (25%)
4	GOL	B	1902	-	5,5,5	0.77	0	5,5,5	0.73	0
4	GOL	B	1904	-	5,5,5	0.80	0	5,5,5	1.83	2 (40%)
3	GCS	B	1903	-	12,12,12	1.31	1 (8%)	16,17,17	2.07	2 (12%)
4	GOL	A	1903	-	5,5,5	0.74	0	5,5,5	0.29	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
3	GCS	A	1902	-	-	0/2/22/22	0/1/1/1
4	GOL	B	1902	-	-	0/4/4/4	-
4	GOL	B	1904	-	-	3/4/4/4	-
3	GCS	B	1903	-	-	0/2/22/22	0/1/1/1
4	GOL	A	1903	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1903	GCS	C1-C2	3.28	1.56	1.52
3	A	1902	GCS	C1-C2	2.01	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1903	GCS	O1-C1-O5	-6.01	92.33	110.38
3	B	1903	GCS	O5-C1-C2	5.10	115.47	109.51
3	A	1902	GCS	O5-C1-C2	4.23	114.44	109.51
3	A	1902	GCS	O1-C1-O5	-4.22	97.72	110.38
3	A	1902	GCS	O5-C5-C4	-3.02	104.20	109.69
4	B	1904	GOL	C3-C2-C1	2.38	120.98	111.70
3	A	1902	GCS	O1-C1-C2	-2.35	104.11	108.96
4	B	1904	GOL	O2-C2-C3	2.09	118.32	109.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1904	GOL	O1-C1-C2-C3
4	B	1904	GOL	O1-C1-C2-O2
4	B	1904	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1902	GCS	1	0
3	B	1903	GCS	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^{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	858/1032 (83%)	-0.31	11 (1%)	77	78	11, 19, 28, 42	1 (0%)
1	B	858/1032 (83%)	-0.28	14 (1%)	72	72	11, 19, 29, 43	0
All	All	1716/2064 (83%)	-0.30	25 (1%)	73	74	11, 19, 29, 43	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	ALA	3.7
1	A	45	GLY	3.2
1	B	830	ARG	3.2
1	A	44	VAL	3.2
1	B	828	GLY	3.1
1	B	581	ASP	2.9
1	B	826	THR	2.7
1	A	47	ALA	2.6
1	A	738	ALA	2.6
1	B	130	ASP	2.6
1	B	827	SER	2.5
1	A	581	ASP	2.5
1	B	259	ASN	2.5
1	B	322	GLY	2.5
1	B	430	GLU	2.5
1	B	321	GLY	2.3
1	A	48	ALA	2.3
1	A	297	ARG	2.3
1	A	43	SER	2.3
1	B	50	ASN	2.2
1	B	46	ALA	2.2
1	A	721	GLY	2.2
1	A	899	ASP	2.2
1	A	259	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	79	SER	2.1

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 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	1899	1/1	0.27	0.73	237,237,237,237	0
2	CD	A	1901	1/1	0.76	0.18	120,120,120,120	0
4	GOL	A	1903	6/6	0.92	0.09	21,22,24,25	0
4	GOL	B	1902	6/6	0.93	0.12	20,24,24,25	0
4	GOL	B	1904	6/6	0.96	0.08	20,20,23,24	0
3	GCS	B	1903	12/12	0.96	0.08	14,16,20,24	0
3	GCS	A	1902	12/12	0.97	0.07	16,18,20,25	0
2	CD	B	1901	1/1	0.97	0.16	76,76,76,76	0
2	CD	A	1900	1/1	0.99	0.13	37,37,37,37	0
2	CD	B	1899	1/1	1.00	0.03	18,18,18,18	0
2	CD	B	1900	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.