



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:07 AM GMT

PDB ID : 2VZV  
Title : SUBSTRATE COMPLEX OF AMYCOLATOPSIS ORIENTALIS EXO-CHITOSANASE CSXA E541A WITH CHITOSAN  
Authors : Lammerts Van Bueren, A.; Ghinet, M.G.; Gregg, K.; Fleury, A.; Brzezinski, R.; Boraston, A.B.  
Deposited on : 2008-08-05  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

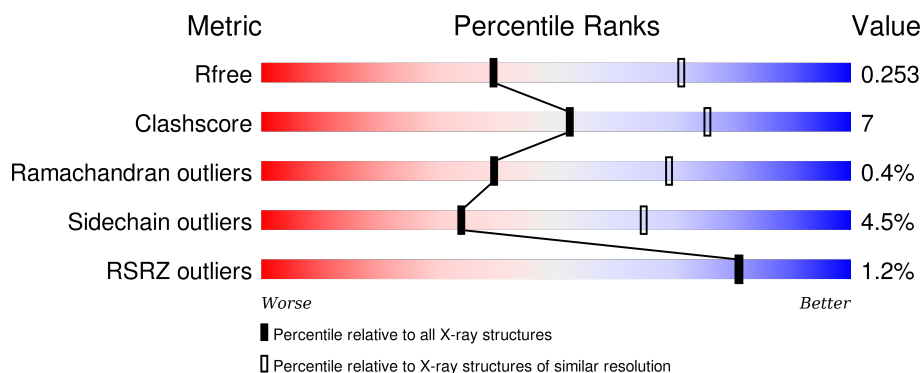
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>70% 13% • 17%</div> </div>
1	B	1032	<div> <div></div> <div>69% 12% • 17%</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
2	GCS	A	1900	-	-	-	X
2	GCS	B	1900	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13565 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
			6548	4113	1133	1285	17			
1	B	858	Total	C	N	O	S	4	0	1
			6548	4113	1133	1285	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	541	ALA	GLU	ENGINEERED MUTATION	UNP Q56F26
A	750	ASN	TRP	CONFLICT	UNP Q56F26
B	541	ALA	GLU	ENGINEERED MUTATION	UNP Q56F26
B	750	ASN	TRP	CONFLICT	UNP Q56F26

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			23	12	2	9		
2	B	2	Total	C	N	O	0	0
			23	12	2	9		

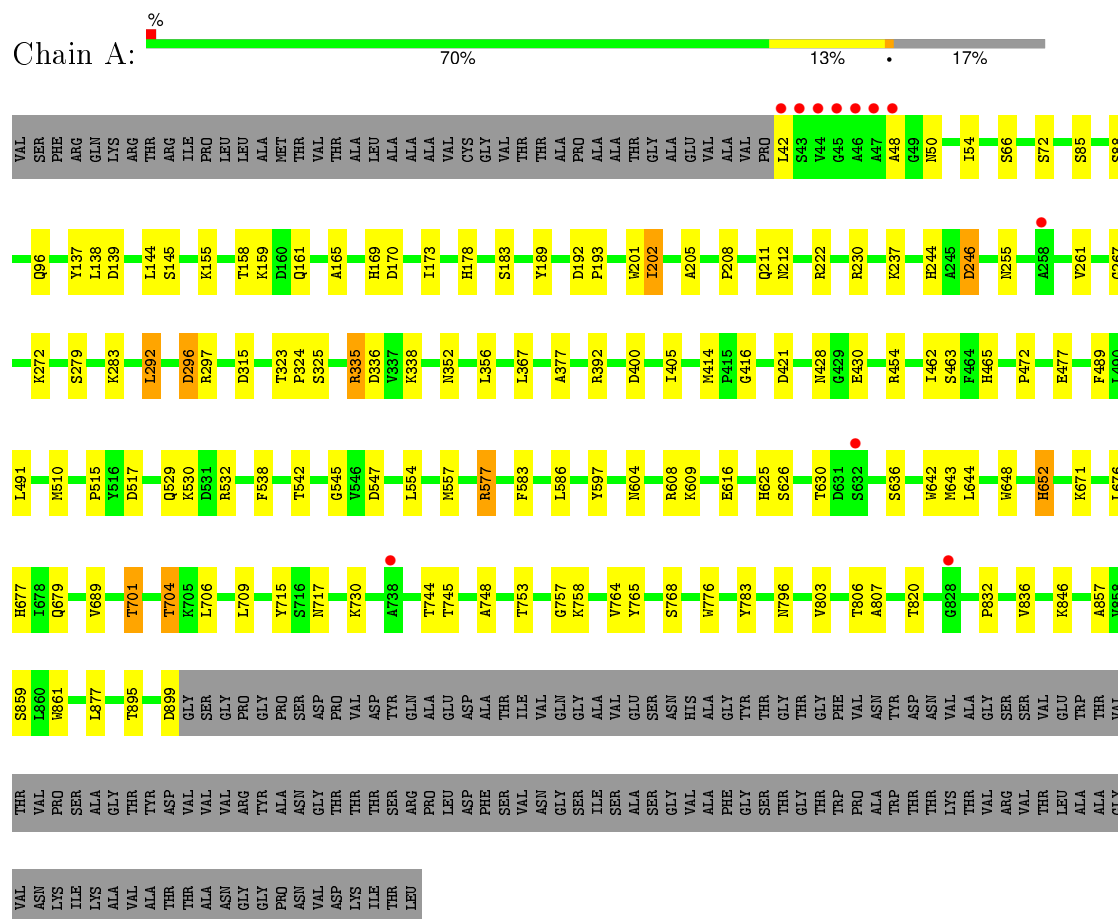
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total	O	0	0
			212	212		
3	B	211	Total	O	0	0
			211	211		

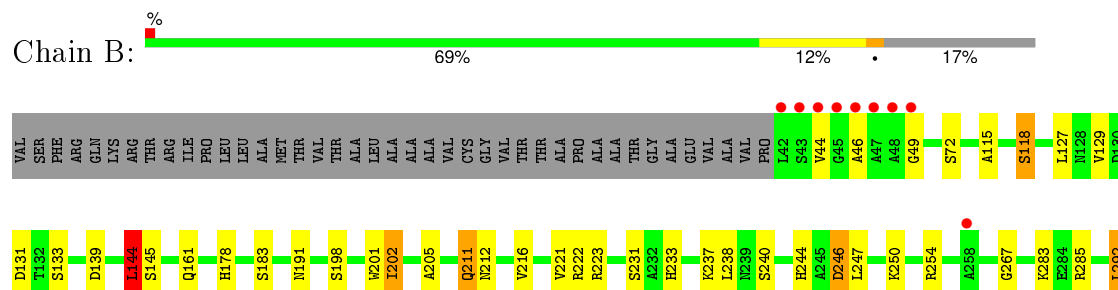
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE



#### • Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE



LVS	ALA	Q894	Y680	L490	D296
VAL	GLY	T895	S681	L491	R297
ALA	TYR	A898	R685	P495	H340
THR	ASP	D899			
THR	VAL	GLY	S688	S502	D315
ALA	VAL	GLY	G699	P503	
ASN	VAL	GLY	L700	L504	T323
GLY	ARG	PRO	T701		T324
GLY	TYR	GLY		K511	
PRO	ALA	PRO	T704	M512	R335
ASN	ASN	ASP			R336
VAL	GLY	ASP	L709	D517	V337
ASP	THR	PRO			
LVS	THR	VAL	V736	P521	N352
ILE	THR	ASP	F737		G353
THR	SER	TYR	A738	K527	K354
LEU	ARG	GLN	W739	S528	P255
	PRO	ALA	W739	Q529	L356
	LEU	GLU	T745		
	ASP	ASP		M536	L369
	PHE	ALA	T753		
	SER	THR	D754	D552	A375
	VAL	ILE			
	VAL	VAL	K758	P570	K379
	GLY	GLN			
	SER	GLY	V764	R577	T390
	ILE	ALA			Y391
	SER	VAL	T769	F583	R392
	ALA	GLU			
	GLY	SER	L774	Y597	G395
	SER	ASN	H775	G598	
	VAL	HIS	W776	A599	D400
	ALA	ALA			
	PHE	GLY	L792	D605	L412
	GLY	TYR			T413
	SER	THR	L798	R608	M414
	THR	GLY			P415
	GLY	THR	V803	D516	G416
	THR	GLY			H417
	TRP	PHE	A807	R627	E418
	PRO	VAL	N808		
	ALA	ASN	S809	D631	N428
	TRP	TYR		S632	G429
	THR	ASP	P832		E430
	THR	ASN			E431
	LVS	VAL	V836		A452
	THR	ALA			E453
	VAL	GLY	R846	M648	R454
	ARG	SER			
	VAL	SER	A857	H652	F464
	THR	VAL	V858		H465
	LEU	THR	S859	F656	
	ALA	TRP	L860	Y659	E477
	ALA	THR	W861	M660	
	GLY	VAL			
	VAL	VAL	T865		M464
	ASN	VAL			
	LVS	THR	L877	H677	M469
	THR	PRO		P678	
	ILE	SER		O679	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.86Å 121.41Å 184.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	185.70 – 2.70 19.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.3 (185.70-2.70) 91.6 (19.97-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.33 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.182 , 0.255 0.184 , 0.253	Depositor DCC
$R_{free}$ test set	2545 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 24.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 49770 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GCS

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	0.54	3/6711 (0.0%)	0.66	5/9158 (0.1%)
1	B	0.52	3/6711 (0.0%)	0.66	8/9158 (0.1%)
All	All	0.53	6/13422 (0.0%)	0.66	13/18316 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	16.66	1.83	1.52
1	B	430	GLU	CB-CG	10.96	1.73	1.52
1	B	246	ASP	CB-CG	7.18	1.66	1.51
1	B	296	ASP	CB-CG	6.59	1.65	1.51
1	A	246	ASP	CB-CG	6.17	1.64	1.51
1	A	296	ASP	CB-CG	5.84	1.64	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ASP	CB-CG-OD1	15.77	132.49	118.30
1	B	246	ASP	CB-CG-OD1	15.13	131.92	118.30
1	B	296	ASP	CB-CG-OD1	14.89	131.71	118.30
1	A	296	ASP	CB-CG-OD2	11.98	129.08	118.30
1	A	430	GLU	CA-CB-CG	-11.08	89.02	113.40
1	A	246	ASP	OD1-CG-OD2	-8.26	107.60	123.30
1	B	246	ASP	OD1-CG-OD2	-7.67	108.73	123.30
1	B	430	GLU	CA-CB-CG	-6.06	100.07	113.40
1	B	247	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	296	ASP	OD1-CG-OD2	-5.59	112.67	123.30
1	B	238	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	296	ASP	OD1-CG-OD2	-5.43	112.97	123.30
1	B	144	LEU	CA-CB-CG	5.31	127.51	115.30



There are no chirality outliers.

There are no planarity outliers.

## 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	6548	0	6327	81	9
1	B	6548	0	6327	92	9
2	A	23	0	23	0	0
2	B	23	0	23	2	0
3	A	212	0	0	9	0
3	B	211	0	0	17	0
All	All	13565	0	12700	173	9

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 (173) 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:201:TRP:HE1	1:B:212:ASN:HD21	1.00	0.93
1:B:310:HIS:CE1	3:B:2079:HOH:O	2.23	0.90
1:B:577:ARG:HG2	1:B:583:PHE:O	1.75	0.85
1:B:244:HIS:HE2	1:B:246:ASP:CG	1.82	0.80
1:B:115:ALA:O	1:B:118:SER:HB2	1.82	0.79
1:A:144:LEU:HD22	1:A:165:ALA:HB2	1.64	0.79
1:B:336:ASP:H	1:B:352:ASN:ND2	1.80	0.78
1:B:310:HIS:CG	3:B:2079:HOH:O	2.39	0.76
1:B:700:LEU:HD23	1:B:754:ASP:HA	1.67	0.75
1:B:310:HIS:HB3	3:B:2082:HOH:O	1.87	0.74
1:B:310:HIS:CD2	3:B:2079:HOH:O	2.40	0.74
1:B:244:HIS:NE2	1:B:246:ASP:OD1	2.15	0.73
1:A:246:ASP:HB3	1:A:292:LEU:HD21	1.72	0.71
1:A:161:GLN:HB2	3:A:2026:HOH:O	1.89	0.71
1:B:178:HIS:HE1	3:B:2043:HOH:O	1.73	0.70
1:A:577:ARG:HG2	1:A:583:PHE:O	1.91	0.70
1:A:400:ASP:OD1	1:A:454:ARG:HD2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ARG:NH1	1:B:736:VAL:O	2.29	0.65
1:B:808:ASN:ND2	1:B:809:SER:H	1.94	0.65
1:B:335:ARG:HH22	1:B:491:LEU:HD21	1.61	0.65
1:B:127:LEU:HD11	1:B:221:VAL:HG21	1.78	0.65
1:B:161:GLN:HB2	3:B:2028:HOH:O	1.95	0.65
1:A:701:THR:HG23	1:A:753:THR:OG1	1.97	0.63
1:B:894:GLN:HB3	3:B:2208:HOH:O	1.98	0.63
1:B:310:HIS:ND1	3:B:2079:HOH:O	2.27	0.63
1:A:178:HIS:HE1	3:A:2033:HOH:O	1.80	0.62
1:A:170:ASP:OD2	1:A:230:ARG:HD2	2.00	0.62
1:A:764:VAL:HG21	1:A:859:SER:HB2	1.81	0.62
1:A:48:ALA:HB1	1:A:325:SER:O	1.99	0.62
1:A:144:LEU:CD2	1:A:165:ALA:HB2	2.29	0.61
1:A:704:THR:HG23	1:A:717:ASN:HB3	1.83	0.60
1:A:489:PHE:CE2	1:A:491:LEU:HB2	2.38	0.59
1:B:400:ASP:OD1	1:B:454:ARG:HD2	2.03	0.59
1:A:201:TRP:HE1	1:A:212:ASN:HD21	1.49	0.59
1:B:529:GLN:HG3	1:B:776:TRP:CE3	2.38	0.58
1:B:310:HIS:NE2	3:B:2079:HOH:O	2.31	0.58
1:B:709:LEU:HD11	1:B:745:THR:HB	1.85	0.58
1:A:709:LEU:HD11	1:A:745:THR:HB	1.86	0.58
1:B:216:VAL:HG11	1:B:369:LEU:HD12	1.86	0.57
1:B:677:HIS:HD2	1:B:679:GLN:HE21	1.52	0.57
1:B:354:LYS:HE3	3:B:2093:HOH:O	2.05	0.56
1:A:577:ARG:NH1	1:A:652:HIS:ND1	2.53	0.56
1:B:511:LYS:HE2	1:B:536:TRP:O	2.05	0.56
1:A:246:ASP:HB3	1:A:292:LEU:CD2	2.34	0.56
1:A:336:ASP:H	1:A:352:ASN:ND2	2.03	0.56
1:A:139:ASP:HA	1:A:169:HIS:O	2.05	0.56
1:A:244:HIS:ND1	1:A:296:ASP:OD1	2.38	0.56
1:A:515:PRO:HD2	1:A:542:THR:OG1	2.06	0.56
1:B:704:THR:HG22	3:B:2180:HOH:O	2.06	0.55
1:A:72:SER:O	1:A:183:SER:HB2	2.07	0.55
1:A:899:ASP:N	3:A:2210:HOH:O	2.40	0.54
1:A:753:THR:HB	1:A:757:GLY:O	2.07	0.54
1:B:244:HIS:NE2	1:B:246:ASP:CG	2.59	0.54
1:A:706:LEU:HB2	1:A:715:TYR:HB3	1.89	0.54
1:B:336:ASP:H	1:B:352:ASN:HD22	1.52	0.54
1:A:836:VAL:O	1:A:857:ALA:HA	2.08	0.54
1:B:495:PRO:HB3	1:B:502:SER:HB3	1.90	0.54
1:B:517:ASP:OD1	1:B:577:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASP:HB3	1:B:292:LEU:HD21	1.89	0.54
1:A:244:HIS:NE2	1:A:246:ASP:CG	2.62	0.54
1:A:244:HIS:NE2	1:A:246:ASP:OD2	2.42	0.53
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.85	0.53
1:A:577:ARG:HD2	1:A:652:HIS:HB3	1.90	0.53
1:B:680:TYR:OH	1:B:685:ARG:HG2	2.09	0.53
1:A:677:HIS:HD2	1:A:679:GLN:HE21	1.55	0.53
1:B:512:MET:HG2	2:B:1900:GCS:H61	1.90	0.53
1:B:808:ASN:HD22	1:B:809:SER:H	1.55	0.53
1:B:803:VAL:O	1:B:894:GLN:NE2	2.36	0.53
1:B:764:VAL:HG21	1:B:859:SER:HB2	1.90	0.52
1:B:375:ALA:O	1:B:379:LYS:HG3	2.10	0.52
1:B:808:ASN:HB3	3:B:2191:HOH:O	2.10	0.51
1:A:155:LYS:HD3	1:A:158:THR:HG22	1.93	0.51
1:A:297:ARG:NH2	3:A:2066:HOH:O	2.43	0.51
1:A:137:TYR:HB2	1:A:222:ARG:HB2	1.92	0.51
1:A:609:LYS:CE	1:A:796:ASN:HD21	2.24	0.50
1:A:244:HIS:NE2	1:A:246:ASP:OD1	2.44	0.50
1:A:465:HIS:HD2	3:A:2120:HOH:O	1.93	0.50
1:A:701:THR:HG23	1:A:753:THR:HG1	1.74	0.50
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.76	0.50
1:A:297:ARG:HD2	3:A:2067:HOH:O	2.12	0.49
1:B:737:PRO:O	1:B:739:VAL:HG23	2.12	0.49
1:A:416:GLY:HA3	1:A:465:HIS:HB2	1.95	0.49
1:A:597:TYR:OH	1:A:616:GLU:OE2	2.21	0.49
1:A:715:TYR:HA	3:A:2173:HOH:O	2.11	0.48
1:A:677:HIS:CD2	1:A:679:GLN:HE21	2.31	0.48
1:A:85:SER:HB3	1:A:96:GLN:HE22	1.78	0.48
1:B:72:SER:O	1:B:183:SER:HB2	2.14	0.48
1:B:836:VAL:O	1:B:857:ALA:HA	2.14	0.48
1:B:465:HIS:HD2	3:B:2124:HOH:O	1.96	0.48
1:B:521:PRO:HG3	1:B:616:GLU:HG2	1.96	0.48
1:A:554:LEU:HA	1:A:557:MET:HG2	1.96	0.48
1:B:677:HIS:CD2	1:B:679:GLN:HE21	2.30	0.47
1:A:392:ARG:HA	1:A:414:MET:HB2	1.96	0.47
1:B:659:TYR:O	1:B:660:MET:HB2	2.14	0.47
1:B:597:TYR:OH	1:B:616:GLU:OE2	2.26	0.47
1:B:161:GLN:CB	3:B:2028:HOH:O	2.58	0.47
1:B:745:THR:HG23	1:B:792:LEU:HA	1.97	0.47
1:B:336:ASP:H	1:B:352:ASN:HD21	1.60	0.47
1:A:193:PRO:O	1:A:421:ASP:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:LEU:HD13	1:B:776:TRP:CZ2	2.51	0.46
1:B:416:GLY:HA3	1:B:465:HIS:HB2	1.97	0.46
1:B:267:GLY:HA3	1:B:315:ASP:O	2.16	0.46
1:A:144:LEU:HA	1:A:145:SER:HA	1.69	0.46
1:B:807:ALA:O	1:B:898:ALA:HA	2.16	0.46
1:B:577:ARG:HD2	1:B:652:HIS:HB3	1.97	0.46
1:A:832:PRO:HB3	1:A:861:TRP:CD2	2.51	0.46
1:A:42:LEU:HD21	1:A:54:ILE:HG12	1.98	0.45
1:B:254:ARG:HG3	1:B:285:ARG:HB2	1.99	0.45
1:B:392:ARG:HA	1:B:414:MET:HB2	1.99	0.45
1:B:129:VAL:HG13	1:B:223:ARG:HH12	1.82	0.45
1:A:159:LYS:HD3	1:A:189:TYR:CZ	2.51	0.45
1:B:477:GLU:HG2	1:B:504:ILE:HD12	1.99	0.45
1:A:255:ASN:ND2	1:A:261:VAL:HG22	2.32	0.45
1:A:529:GLN:HG3	1:A:776:TRP:CE3	2.51	0.45
1:B:709:LEU:HD22	1:B:798:LEU:HD13	1.99	0.45
1:A:517:ASP:OD1	1:A:577:ARG:NH2	2.50	0.45
1:B:395:GLY:HA3	1:B:418:GLU:OE1	2.17	0.45
1:A:472:PRO:HG2	1:A:477:GLU:HB2	1.99	0.45
1:B:570:PRO:HD2	3:B:2145:HOH:O	2.17	0.44
1:B:46:ALA:HB2	1:B:131:ASP:HB3	1.98	0.44
1:A:701:THR:HG22	3:A:2177:HOH:O	2.16	0.44
1:A:336:ASP:OD1	1:A:338:LYS:NZ	2.50	0.44
1:A:642:TRP:CD2	1:A:643:MET:HG2	2.53	0.44
1:A:201:TRP:O	1:A:202:ILE:C	2.56	0.44
1:A:547:ASP:H	1:A:652:HIS:HA	1.82	0.43
1:B:310:HIS:CD2	3:B:2082:HOH:O	2.71	0.43
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.83	0.43
1:B:656:PHE:CE1	1:B:660:MET:HE1	2.53	0.43
1:B:512:MET:HG2	2:B:1900:GCS:C6	2.47	0.43
1:A:689:VAL:O	1:A:730:LYS:HA	2.19	0.43
1:B:753:THR:HA	1:B:758:LYS:O	2.18	0.43
1:A:625:HIS:O	1:A:636:SER:OG	2.35	0.43
1:B:627:ARG:NH1	1:B:681:SER:HB3	2.33	0.43
1:A:144:LEU:CD2	1:A:165:ALA:CB	2.95	0.43
1:B:44:VAL:HG21	1:B:221:VAL:HG11	2.00	0.43
1:B:233:HIS:CE1	1:B:250:LYS:HB2	2.54	0.43
1:A:748:ALA:HB3	1:A:765:TYR:HB2	2.00	0.43
1:A:642:TRP:HA	1:A:643:MET:HA	1.66	0.42
1:B:139:ASP:OD2	1:B:222:ARG:NH1	2.51	0.42
1:A:462:ILE:O	1:A:463:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ARG:NH2	1:B:491:LEU:HD21	2.31	0.42
1:A:208:PRO:HD3	1:A:367:LEU:HD11	2.00	0.42
1:B:390:THR:HA	1:B:412:LEU:O	2.20	0.42
1:A:50:ASN:C	1:A:50:ASN:OD1	2.57	0.42
1:B:527:LYS:NZ	1:B:631:ASP:OD2	2.47	0.42
1:A:517:ASP:HA	1:A:545:GLY:HA3	2.01	0.42
1:A:671:LYS:HE2	1:A:671:LYS:HB2	1.95	0.42
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.85	0.42
1:A:267:GLY:HA3	1:A:315:ASP:O	2.20	0.42
1:B:464:PHE:HB3	1:B:484:MET:HE1	2.01	0.42
1:B:201:TRP:O	1:B:202:ILE:C	2.57	0.42
1:A:832:PRO:HB3	1:A:861:TRP:CE2	2.55	0.42
1:B:701:THR:HG23	1:B:753:THR:OG1	2.21	0.41
1:B:129:VAL:HG13	1:B:223:ARG:NH1	2.35	0.41
1:A:323:THR:HG22	1:A:324:PRO:O	2.21	0.41
1:B:428:ASN:HB2	1:B:431:GLU:HB3	2.03	0.41
1:B:865:THR:HG22	3:B:2201:HOH:O	2.20	0.41
1:B:452:ALA:HB1	1:B:489:PHE:HB2	2.02	0.41
1:B:642:TRP:HA	1:B:643:MET:HA	1.77	0.41
1:B:144:LEU:N	1:B:144:LEU:HD23	2.35	0.41
1:B:605:ASP:HA	1:B:608:ARG:HD3	2.03	0.41
1:A:807:ALA:HA	1:A:820:THR:O	2.21	0.41
1:A:377:ALA:HA	1:A:405:ILE:HG21	2.02	0.41
1:B:191:ASN:O	1:B:211:GLN:HG2	2.20	0.41
1:A:604:ASN:HB3	3:A:2148:HOH:O	2.19	0.41
1:A:744:THR:O	1:A:768:SER:HA	2.21	0.41
1:B:144:LEU:HA	1:B:145:SER:HA	1.69	0.41
1:A:532:ARG:HA	1:A:532:ARG:HD3	1.97	0.41
1:A:510:MET:HA	1:A:538:PHE:HB3	2.03	0.41
1:B:323:THR:HA	1:B:324:PRO:HD2	1.94	0.40
1:B:495:PRO:CB	1:B:502:SER:HB3	2.51	0.40
1:B:832:PRO:HB3	1:B:861:TRP:CE2	2.57	0.40
1:A:138:LEU:HG	1:A:173:ILE:HD13	2.04	0.40

All (9) 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)
1:A:246:ASP:OD2	1:B:296:ASP:OD1[3_554]	1.58	0.62
1:A:296:ASP:OD2	1:B:246:ASP:OD1[3_554]	1.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASP:OD2	1:B:246:ASP:OD2[3_554]	1.61	0.59
1:A:246:ASP:OD1	1:B:296:ASP:OD1[3_554]	1.75	0.45
1:A:246:ASP:OD2	1:B:296:ASP:CG[3_554]	1.82	0.38
1:A:296:ASP:OD2	1:B:246:ASP:CG[3_554]	1.85	0.35
1:A:296:ASP:CG	1:B:246:ASP:OD2[3_554]	2.02	0.18
1:A:246:ASP:CG	1:B:296:ASP:OD1[3_554]	2.06	0.14
1:A:246:ASP:OD2	1:B:296:ASP:OD2[3_554]	2.14	0.06

## 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%)	811 (95%)	42 (5%)	3 (0%)	39	69
1	B	856/1032 (83%)	810 (95%)	42 (5%)	4 (0%)	34	63
All	All	1712/2064 (83%)	1621 (95%)	84 (5%)	7 (0%)	39	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	LYS
1	B	202	ILE
1	A	202	ILE
1	A	205	ALA
1	B	205	ALA
1	B	599	ALA
1	B	49	GLY

### 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	701/833 (84%)	672 (96%)	29 (4%)	37	69
1	B	701/833 (84%)	667 (95%)	34 (5%)	31	61
All	All	1402/1666 (84%)	1339 (96%)	63 (4%)	34	65

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	88	SER
1	A	211	GLN
1	A	237	LYS
1	A	272	LYS
1	A	279	SER
1	A	283	LYS
1	A	292	LEU
1	A	335	ARG
1	A	356	LEU
1	A	428	ASN
1	A	530	LYS
1	A	577	ARG
1	A	586	LEU
1	A	608	ARG
1	A	626	SER
1	A	630	THR
1	A	644	LEU
1	A	648	TRP
1	A	652	HIS
1	A	676	LEU
1	A	701	THR
1	A	704	THR
1	A	783	TYR
1	A	803	VAL
1	A	806	THR
1	A	846	LYS
1	A	877	LEU
1	A	895	THR
1	B	118	SER
1	B	133	SER
1	B	144	LEU
1	B	198	SER

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Mol	Chain	Res	Type
1	B	211	GLN
1	B	231	SER
1	B	237	LYS
1	B	240	SER
1	B	283	LYS
1	B	292	LEU
1	B	297	ARG
1	B	310	HIS
1	B	324	PRO
1	B	335	ARG
1	B	337	VAL
1	B	356	LEU
1	B	428	ASN
1	B	517	ASP
1	B	552	ASP
1	B	577	ARG
1	B	608	ARG
1	B	632	SER
1	B	648	TRP
1	B	652	HIS
1	B	698	SER
1	B	701	THR
1	B	704	THR
1	B	769	THR
1	B	803	VAL
1	B	808	ASN
1	B	846	LYS
1	B	865	THR
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	96	GLN
1	A	178	HIS
1	A	194	ASN
1	A	212	ASN
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	478	GLN

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Mol	Chain	Res	Type
1	A	679	GLN
1	A	750	ASN
1	A	796	ASN
1	B	128	ASN
1	B	169	HIS
1	B	178	HIS
1	B	194	ASN
1	B	212	ASN
1	B	310	HIS
1	B	352	ASN
1	B	428	ASN
1	B	465	HIS
1	B	679	GLN
1	B	750	ASN
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 ⓘ

4 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GCS	A	1899	2	11,11,12	0.57	0	13,15,17	1.51	2 (15%)
2	GCS	A	1900	2	12,12,12	1.66	4 (33%)	15,17,17	1.39	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GCS	B	1899	2	11,11,12	0.77	0	13,15,17	1.98	2 (15%)
2	GCS	B	1900	2	12,12,12	1.37	1 (8%)	15,17,17	1.50	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GCS	A	1899	2	-	0/2/19/22	0/1/1/1
2	GCS	A	1900	2	-	0/2/22/22	0/1/1/1
2	GCS	B	1899	2	-	0/2/19/22	0/1/1/1
2	GCS	B	1900	2	-	0/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1900	GCS	C6-C5	2.08	1.59	1.51
2	A	1900	GCS	C4-C5	2.12	1.57	1.53
2	A	1900	GCS	O5-C5	2.25	1.50	1.44
2	B	1900	GCS	O4-C4	2.71	1.49	1.43
2	A	1900	GCS	O4-C4	2.72	1.49	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1899	GCS	O5-C5-C6	-2.68	101.55	107.35
2	B	1899	GCS	C4-C3-C2	-2.30	108.28	111.39
2	B	1900	GCS	C6-C5-C4	-2.05	107.95	113.02
2	A	1900	GCS	O5-C5-C4	2.21	113.83	109.68
2	A	1900	GCS	O1-C1-C2	2.43	114.55	109.02
2	A	1900	GCS	O4-C4-C3	2.59	116.17	110.34
2	A	1899	GCS	C1-O5-C5	3.82	117.09	112.25
2	B	1900	GCS	O5-C5-C4	4.39	117.92	109.68
2	B	1899	GCS	C1-O5-C5	6.26	120.19	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1900	GCS	2	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	858/1032 (83%)	-0.42	11 (1%) 79 79	3, 15, 27, 66	1 (0%)
1	B	858/1032 (83%)	-0.41	10 (1%) 81 81	3, 15, 25, 68	1 (0%)
All	All	1716/2064 (83%)	-0.42	21 (1%) 81 81	3, 15, 26, 68	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	SER	7.8
1	A	47	ALA	6.3
1	A	44	VAL	6.0
1	A	45	GLY	5.9
1	B	46	ALA	5.6
1	B	45	GLY	5.4
1	B	44	VAL	5.1
1	A	42	LEU	4.5
1	A	43	SER	4.3
1	B	258	ALA	3.5
1	B	42	LEU	3.4
1	B	47	ALA	3.2
1	A	46	ALA	3.1
1	A	632	SER	3.0
1	B	48	ALA	2.8
1	A	828	GLY	2.7
1	A	738	ALA	2.4
1	A	258	ALA	2.3
1	A	48	ALA	2.2
1	B	429	GLY	2.1
1	B	49	GLY	2.1

## 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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GCS	B	1900	12/12	0.90	0.20	2.72	28,33,34,35	0
2	GCS	A	1900	12/12	0.88	0.20	2.68	26,28,28,29	0
2	GCS	B	1899	11/12	0.94	0.15	1.56	19,22,23,24	0
2	GCS	A	1899	11/12	0.96	0.15	1.01	15,19,21,22	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.