



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:14 AM GMT

PDB ID : 2X05  
Title : INHIBITION OF THE EXO-BETA-D-GLUCOSAMINIDASECSXA BY A  
GLUCOSAMINE-CONFIGUREDCASTANOSPERMINE AND AN AMINO-  
AUSTRALINE ANALOGUE  
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Deposited on : 2009-12-05  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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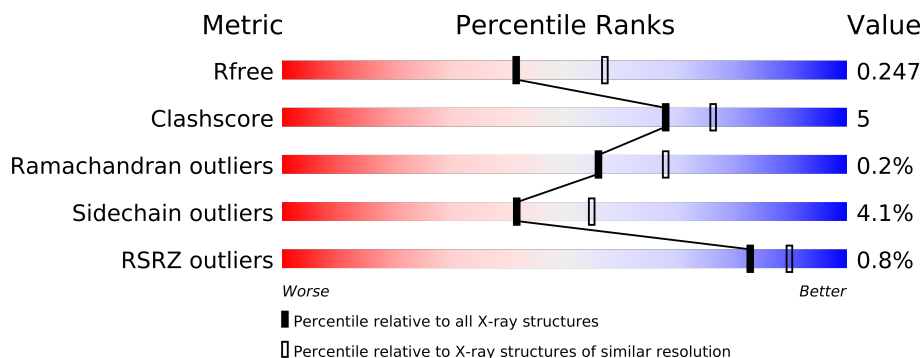
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1032	
1	B	1032	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CD	A	1907	-	X
3	CD	A	1908	-	X
3	CD	B	1903	-	X
3	CD	B	1904	-	X
3	CD	B	1905	-	X
3	CD	B	1906	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	CD	B	1907	-	X
3	CD	B	1908	-	X
3	CD	B	1909	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14302 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

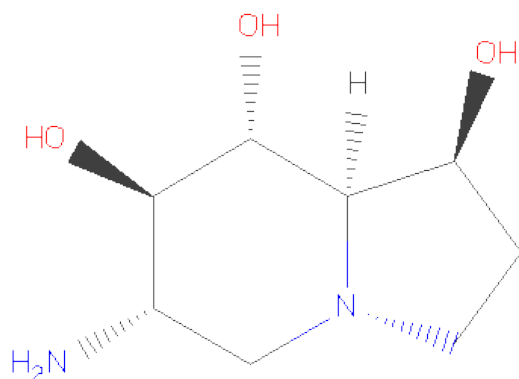
- Molecule 1 is a protein called EXO-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	4	1	1
			6520	4095	1127	1281	17			
1	B	852	Total	C	N	O	S	0	3	1
			6532	4104	1128	1282	18			

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 AMINO-CASTANOSPERMINE (three-letter code: X05) (formula: C<sub>8</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	8	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			13	8	2	3		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	10	Total	Cd	0	0
			10	10		
3	A	9	Total	Cd	0	0
			9	9		

- Molecule 4 is water.

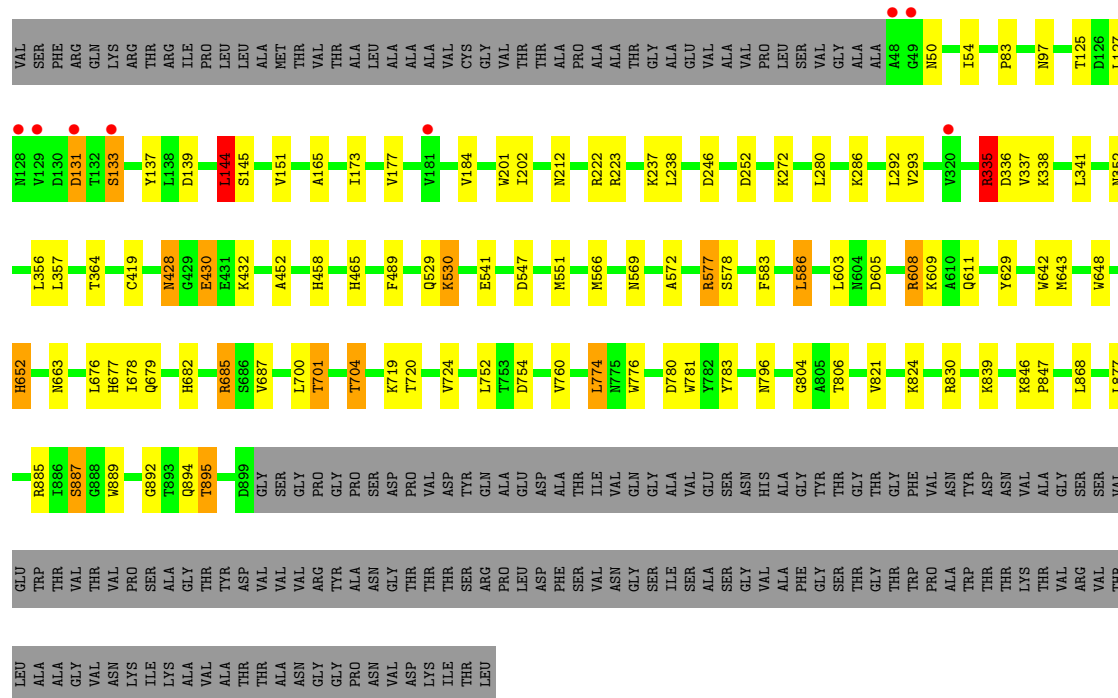
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	604	Total	O	0	0
			604	604		
4	B	601	Total	O	0	0
			601	601		

### 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.

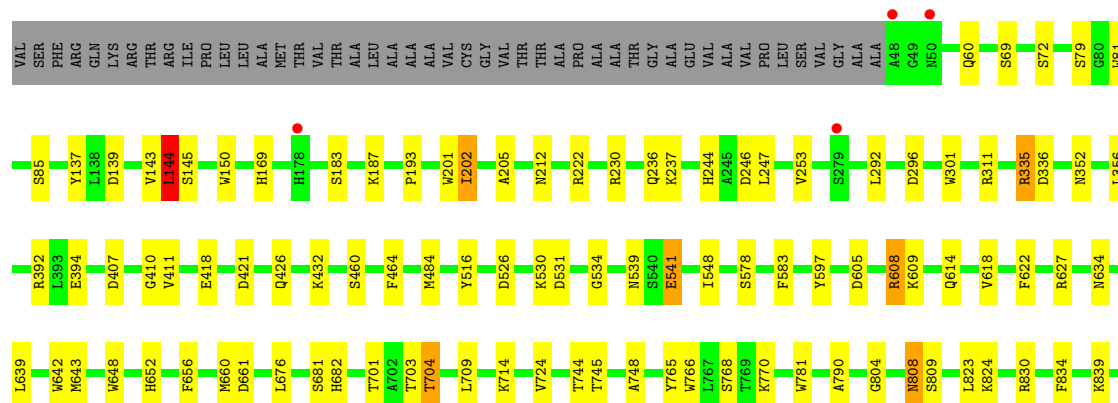
#### • Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain A: 



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

Chain B: 



K846	P847	Y848	L877	S880	W889	T895	D899	GLY	SER	GLY	PRO	GLY	PRO	SER	ASP	PRO	VAL	THR	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	THR	VAL	GLY	SER	SER	VAL
LEU	ALA	ALA	GLY	VAL	ASN	LYS	ILE	LYS	ALA	VAL	ALA	THR	THR	THR	THR	THR	THR	THR	THR	SER	ARG	GLN	PRO	LEU	ASP	PHE	SER	SER	VAL	ASN	GLY	ILE	SER	ALA	SER	GLY	VAL	PHE	GLY	THR	THR	THR	GLY	THR	TRP	PRO	ALA	TYR	THR	THR	THR	LYS	THR	VAL	ARG	VAL	THR
LEU	ALA	ALA	GLY	VAL	ASN	LYS	ILE	LYS	ALA	VAL	ALA	THR	THR	THR	THR	THR	THR	THR	THR	SER	ARG	GLN	PRO	LEU	ASP	PHE	SER	SER	VAL	ASN	GLY	ILE	SER	ALA	SER	GLY	VAL	PHE	GLY	THR	THR	THR	GLY	THR	TRP	PRO	ALA	TYR	THR	THR	THR	LYS	THR	VAL	ARG	VAL	THR

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.12Å 121.80Å 91.56Å 90.00° 90.51° 90.00°	Depositor
Resolution (Å)	43.79 – 2.30 43.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.79-2.30) 99.0 (43.79-2.30)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.184 , 0.248 0.185 , 0.247	Depositor DCC
$R_{free}$ test set	4151 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 11.6	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83006 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: X05, 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	0.57	1/6686 (0.0%)	0.68	3/9123 (0.0%)
1	B	0.56	0/6701	0.68	4/9143 (0.0%)
All	All	0.57	1/13387 (0.0%)	0.68	7/18266 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	13.47	1.77	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	GLU	CA-CB-CG	-7.71	96.45	113.40
1	B	230	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	144	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	335	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	144	LEU	CA-CB-CG	5.15	127.16	115.30
1	B	335	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	392	ARG	NE-CZ-NH2	-5.11	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6520	0	6295	65	0
1	B	6532	0	6312	60	3
2	A	13	0	16	4	0
2	B	13	0	16	5	0
3	A	9	0	0	0	3
3	B	10	0	0	0	0
4	A	604	0	0	7	0
4	B	601	0	0	9	0
All	All	14302	0	12639	125	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (125) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:TRP:HE1	1:B:212:ASN:HD21	1.03	1.01
1:A:246:ASP:HB3	1:A:292:LEU:HD11	1.53	0.91
1:A:608:ARG:HG3	1:A:889:TRP:CZ3	2.07	0.90
1:A:201:TRP:HE1	1:A:212:ASN:ND2	1.69	0.90
1:A:541:GLU:OE1	2:A:1900:X05:HAG2	1.76	0.84
1:A:577:ARG:HG2	1:A:583:PHE:O	1.76	0.84
1:B:246:ASP:HB3	1:B:292:LEU:HD11	1.59	0.83
1:B:608:ARG:HG3	1:B:889:TRP:CZ3	2.15	0.81
1:A:139:ASP:OD2	1:A:222:ARG:NH1	2.17	0.77
1:B:531:ASP:HB2	4:B:2385:HOH:O	1.84	0.77
1:B:336:ASP:H	1:B:352:ASN:ND2	1.85	0.73
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.85	0.69
1:A:201:TRP:HE1	1:A:212:ASN:HD21	0.85	0.69
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.58	0.69
1:B:311:ARG:HD3	4:B:2302:HOH:O	1.92	0.68
1:B:311:ARG:HD2	1:B:407:ASP:HB3	1.77	0.66
1:B:605:ASP:HA	1:B:608:ARG:HD3	1.77	0.65
1:A:458:HIS:NE2	4:A:2341:HOH:O	2.30	0.65
1:A:846:LYS:HD3	1:A:847:PRO:HD2	1.79	0.62
1:A:821:VAL:HG13	1:A:868:LEU:HB2	1.81	0.62
1:A:701:THR:HB	1:A:720:THR:HA	1.83	0.61
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.67	0.59
1:A:566:MET:HG3	1:A:586:LEU:HD11	1.84	0.59
1:A:577:ARG:HD2	1:A:652:HIS:ND1	2.18	0.58
1:B:139:ASP:OD2	1:B:222:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:541:GLU:OE2	2:A:1900:X05:NAA	2.37	0.58
1:A:577:ARG:HD2	1:A:652:HIS:CG	2.39	0.58
1:A:685:ARG:HB2	1:A:685:ARG:HH11	1.70	0.57
1:A:419:CYS:SG	2:A:1900:X05:HAH	2.45	0.57
1:A:137:TYR:HB2	1:A:222:ARG:HB2	1.86	0.57
1:A:530:LYS:HG3	4:A:2384:HOH:O	2.05	0.57
1:B:804:GLY:HA3	1:B:824:LYS:O	2.06	0.56
1:A:578:SER:HB3	1:A:583:PHE:O	2.06	0.56
1:B:193:PRO:O	1:B:421:ASP:HB2	2.06	0.55
1:B:187:LYS:NZ	4:B:2113:HOH:O	2.10	0.55
1:A:336:ASP:H	1:A:352:ASN:ND2	2.04	0.55
1:A:682:HIS:HE1	4:A:2438:HOH:O	1.90	0.54
1:B:714:LYS:HE3	4:B:2492:HOH:O	2.08	0.54
1:A:804:GLY:HA3	1:A:824:LYS:O	2.08	0.54
1:B:808:ASN:HD22	1:B:809:SER:H	1.58	0.52
1:B:139:ASP:HA	1:B:169:HIS:O	2.10	0.52
1:B:597:TYR:O	1:B:609:LYS:HE2	2.10	0.52
1:A:839:LYS:HE2	4:A:2460:HOH:O	2.10	0.52
1:B:766:TRP:CE3	1:B:834:PHE:HZ	2.28	0.52
1:B:426:GLN:O	1:B:426:GLN:HG3	2.10	0.51
1:A:83:PRO:HD2	1:A:97:ASN:OD1	2.11	0.51
1:B:704:THR:CG2	4:B:2485:HOH:O	2.58	0.51
1:B:622:PHE:CD1	1:B:639:LEU:HD23	2.46	0.51
1:B:661:ASP:OD1	1:B:839:LYS:NZ	2.42	0.50
1:A:428:ASN:ND2	4:A:2316:HOH:O	2.45	0.49
1:B:877:LEU:HG	1:B:880:SER:O	2.13	0.49
1:A:529:GLN:HG3	1:A:776:TRP:CE3	2.48	0.49
1:A:144:LEU:HD22	1:A:165:ALA:HB2	1.93	0.48
1:B:201:TRP:O	1:B:202:ILE:C	2.51	0.48
1:A:821:VAL:CG1	1:A:868:LEU:HB2	2.44	0.48
1:B:578:SER:HB3	1:B:583:PHE:O	2.13	0.48
1:A:144:LEU:HD22	1:A:165:ALA:CB	2.43	0.48
1:B:246:ASP:CB	1:B:292:LEU:HD11	2.38	0.47
1:B:804:GLY:O	1:B:823:LEU:HA	2.14	0.47
1:B:394:GLU:HG2	1:B:418:GLU:HA	1.95	0.47
1:B:411:VAL:O	1:B:460:SER:HB2	2.14	0.47
1:A:50:ASN:HB3	1:A:223:ARG:HB2	1.97	0.47
1:B:704:THR:HG22	4:B:2485:HOH:O	2.14	0.47
1:A:687:VAL:HG21	1:A:704:THR:HG21	1.97	0.47
1:B:526:ASP:O	1:B:534:GLY:HA3	2.15	0.46
1:A:54:ILE:HG21	1:A:125:THR:HG21	1.98	0.46
1:A:781:TRP:HZ3	2:A:1900:X05:HAE1	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:781:TRP:CZ3	2:B:1900:X05:HAE1	2.51	0.46
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.97	0.46
1:B:137:TYR:HB2	1:B:222:ARG:HB2	1.98	0.45
1:B:614:GLN:O	1:B:618:VAL:HG23	2.16	0.45
1:B:682:HIS:HE1	4:B:2445:HOH:O	1.99	0.45
1:B:848:VAL:HG21	1:B:877:LEU:CD1	2.46	0.45
1:B:744:THR:O	1:B:768:SER:HA	2.16	0.45
1:B:541:GLU:OE1	2:B:1900:X05:HAG2	2.16	0.45
1:B:781:TRP:HZ3	2:B:1900:X05:HAE1	1.82	0.45
1:A:611:GLN:OE1	1:A:663:ASN:HB2	2.16	0.45
1:A:357:LEU:HB2	1:A:629:TYR:CD1	2.51	0.45
1:B:541:GLU:OE2	2:B:1900:X05:NAA	2.50	0.44
1:A:887:SER:HA	1:A:892:GLY:O	2.18	0.44
1:B:899:ASP:N	4:B:2600:HOH:O	2.51	0.44
1:B:418:GLU:OE2	1:B:421:ASP:OD2	2.35	0.44
1:A:338:LYS:HD2	4:A:2259:HOH:O	2.17	0.44
1:B:516:TYR:CZ	2:B:1900:X05:HAF2	2.52	0.44
1:B:301:TRP:CZ2	1:B:410:GLY:HA2	2.53	0.44
1:B:709:LEU:HG	1:B:745:THR:O	2.18	0.44
1:A:577:ARG:CG	1:A:583:PHE:O	2.59	0.43
1:B:464:PHE:HB3	1:B:484:MET:HE1	2.01	0.43
1:A:131:ASP:OD2	1:A:133:SER:HB2	2.19	0.43
1:A:151:VAL:HG22	1:A:184:VAL:HG22	2.01	0.43
1:B:748:ALA:HB3	1:B:765:TYR:HB2	2.01	0.43
1:B:656:PHE:CE1	1:B:660[A]:MET:HE1	2.54	0.42
1:B:642:TRP:HA	1:B:643:MET:HA	1.79	0.42
1:A:605:ASP:HA	1:A:608:ARG:HD3	2.00	0.42
1:A:609:LYS:NZ	1:A:796:ASN:HD21	2.17	0.42
1:B:72:SER:O	1:B:183:SER:HB2	2.19	0.42
1:A:677:HIS:HD2	1:A:679:GLN:HE21	1.66	0.42
1:A:272:LYS:HG3	1:A:293:VAL:HG11	2.00	0.42
1:A:144:LEU:HA	1:A:145:SER:HA	1.80	0.42
1:B:770:LYS:O	1:B:790:ALA:HA	2.20	0.42
1:A:608:ARG:HG3	1:A:889:TRP:HZ3	1.74	0.41
1:B:548:ILE:H	1:B:614:GLN:NE2	2.18	0.41
1:B:627:ARG:NH1	1:B:681:SER:HB3	2.36	0.41
1:A:569:ASN:ND2	1:A:572:ALA:HB2	2.35	0.41
1:A:676:LEU:HD23	1:A:760:VAL:HG21	2.03	0.41
1:A:608:ARG:HG3	1:A:889:TRP:CH2	2.54	0.41
1:A:885:ARG:HG3	1:A:895:THR:HG22	2.01	0.41
1:B:656:PHE:CD1	1:B:660[A]:MET:HE1	2.55	0.41
1:A:252:ASP:HA	1:A:286:LYS:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:701:THR:HA	1:A:719:LYS:O	2.20	0.41
1:A:551:MET:HE1	1:A:603:LEU:HG	2.02	0.41
1:B:703:THR:HG22	4:B:2522:HOH:O	2.21	0.41
1:B:60:GLN:HB2	1:B:81:TRP:CD2	2.55	0.41
1:A:700:LEU:HD23	1:A:754:ASP:HA	2.03	0.41
1:A:642:TRP:CD2	1:A:643:MET:HG2	2.55	0.41
1:B:530:LYS:O	1:B:530:LYS:HD2	2.20	0.41
1:A:144:LEU:N	1:A:144:LEU:HD23	2.36	0.40
1:A:173:ILE:O	1:A:177:VAL:HG23	2.21	0.40
1:A:774:LEU:HD13	1:A:776:TRP:CZ2	2.56	0.40
1:A:280:LEU:HD21	1:A:286:LYS:HB2	2.01	0.40
1:A:547:ASP:H	1:A:652:HIS:HA	1.87	0.40
1:B:144:LEU:HA	1:B:145:SER:HA	1.68	0.40
1:A:678:ILE:HB	1:A:752:LEU:HB2	2.03	0.40
1:B:69:SER:HA	1:B:150:TRP:CZ3	2.55	0.40
1:A:465:HIS:HD2	4:A:2343:HOH:O	2.04	0.40

All (3) 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	Distance(Å)	Clash(Å)
1:B:246:ASP:OD1	3:A:1902:CD:CD[2.557]	1.99	0.21
1:B:244:HIS:NE2	3:A:1902:CD:CD[2.557]	2.09	0.11
1:B:296:ASP:OD2	3:A:1905:CD:CD[2.557]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	851/1032 (82%)	824 (97%)	26 (3%)	1 (0%)	59	72
1	B	853/1032 (83%)	817 (96%)	33 (4%)	3 (0%)	43	52
All	All	1704/2064 (83%)	1641 (96%)	59 (4%)	4 (0%)	56	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ILE
1	B	202	ILE
1	B	541	GLU
1	B	205	ALA

### 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	700/834 (84%)	667 (95%)	33 (5%)	36	47
1	B	702/834 (84%)	678 (97%)	24 (3%)	49	64
All	All	1402/1668 (84%)	1345 (96%)	57 (4%)	41	55

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	131	ASP
1	A	133	SER
1	A	144	LEU
1	A	237	LYS
1	A	238	LEU
1	A	335	ARG
1	A	337	VAL
1	A	341	LEU
1	A	356	LEU
1	A	364	THR
1	A	428	ASN
1	A	430	GLU
1	A	432	LYS
1	A	530	LYS
1	A	577	ARG
1	A	586	LEU
1	A	608	ARG
1	A	648	TRP
1	A	652	HIS
1	A	685	ARG
1	A	701	THR

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Mol	Chain	Res	Type
1	A	704	THR
1	A	724	VAL
1	A	774	LEU
1	A	780	ASP
1	A	783	TYR
1	A	806	THR
1	A	830	ARG
1	A	877	LEU
1	A	887	SER
1	A	894	GLN
1	A	895	THR
1	B	79	SER
1	B	85	SER
1	B	143	VAL
1	B	144	LEU
1	B	236	GLN
1	B	237	LYS
1	B	247	LEU
1	B	253	VAL
1	B	356	LEU
1	B	432	LYS
1	B	539	ASN
1	B	608	ARG
1	B	634	ASN
1	B	648	TRP
1	B	652	HIS
1	B	676	LEU
1	B	701	THR
1	B	704	THR
1	B	724	VAL
1	B	808	ASN
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	194	ASN
1	A	212	ASN

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Mol	Chain	Res	Type
1	A	262	GLN
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	529	GLN
1	A	679	GLN
1	A	682	HIS
1	A	750	ASN
1	A	796	ASN
1	A	808	ASN
1	B	128	ASN
1	B	176	GLN
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	750	ASN
1	B	796	ASN
1	B	808	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 19 are monoatomic - leaving 2 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	$\# Z  > 2$
2	X05	A	1900	-	14,14,14	1.07	1 (7%)	21,21,21	1.36	2 (9%)
2	X05	B	1900	-	14,14,14	0.92	0	21,21,21	1.55	3 (14%)

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	X05	A	1900	-	-	0/0/29/29	0/0/2/2
2	X05	B	1900	-	-	0/0/29/29	0/0/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1900	X05	CAI-CAL	-2.17	1.52	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1900	X05	CAI-CAL-CAK	-3.74	111.88	117.24
2	A	1900	X05	CAI-CAL-CAK	-3.67	111.98	117.24
2	B	1900	X05	CAI-CAL-NAM	-3.32	100.57	104.67
2	A	1900	X05	CAE-CAI-CAL	-2.89	99.95	102.63
2	B	1900	X05	CAG-CAH-CAJ	2.68	113.86	109.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	852/1032 (82%)	-0.23	8 (0%) 81 88	8, 18, 28, 47	1 (0%)
1	B	852/1032 (82%)	-0.28	4 (0%) 88 94	8, 18, 27, 42	0
All	All	1704/2064 (82%)	-0.26	12 (0%) 83 91	8, 18, 28, 47	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	3.7
1	A	49	GLY	3.0
1	A	48	ALA	2.8
1	B	178	HIS	2.5
1	A	128	ASN	2.3
1	A	181	VAL	2.3
1	A	131	ASP	2.2
1	B	279	SER	2.2
1	A	133	SER	2.1
1	B	50	ASN	2.0
1	A	129	VAL	2.0
1	A	320	VAL	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CD	B	1904	1/1	0.23	14.13	97,97,97,97	0
3	CD	A	1908	1/1	0.24	9.01	169,169,169,169	0
3	CD	B	1905	1/1	0.24	6.55	93,93,93,93	0
3	CD	B	1907	1/1	0.20	6.21	139,139,139,139	0
3	CD	A	1907	1/1	0.16	3.37	118,118,118,118	0
3	CD	B	1909	1/1	0.15	2.95	112,112,112,112	0
3	CD	B	1906	1/1	0.18	2.84	132,132,132,132	0
3	CD	B	1903	1/1	0.17	2.77	93,93,93,93	0
3	CD	B	1908	1/1	0.14	2.19	146,146,146,146	0
3	CD	A	1906	1/1	0.19	1.91	116,116,116,116	0
2	X05	B	1900	13/13	0.16	1.64	15,16,18,19	0
3	CD	B	1902	1/1	0.12	1.47	60,60,60,60	0
2	X05	A	1900	13/13	0.15	1.19	14,17,20,21	0
3	CD	B	1910	1/1	0.14	1.03	154,154,154,154	0
3	CD	B	1901	1/1	0.09	-0.94	69,69,69,69	0
3	CD	A	1904	1/1	0.09	-1.16	76,76,76,76	0
3	CD	A	1903	1/1	0.09	-2.05	60,60,60,60	0
3	CD	A	1902	1/1	0.01	-3.38	11,11,11,11	0
3	CD	A	1901	1/1	0.03	-4.27	29,29,29,29	0
3	CD	A	1905	1/1	0.01	-5.93	12,12,12,12	0
3	CD	A	1909	1/1	0.02	-6.15	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.