Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:43 pm GMT

PDB ID	:	2X09
Title	:	Inhibition of the exo-beta-D-glucosaminidase CsxA by a glucosamine- configured castanospermine and an amino-australine analogue
Authors	:	Pluvinage, B.; Ghinet, M.G.; Brzezinski, R.; Boraston, A.B.; Stubbs, K.A.
Deposited on	:	2009-12-07
Resolution	:	2.40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

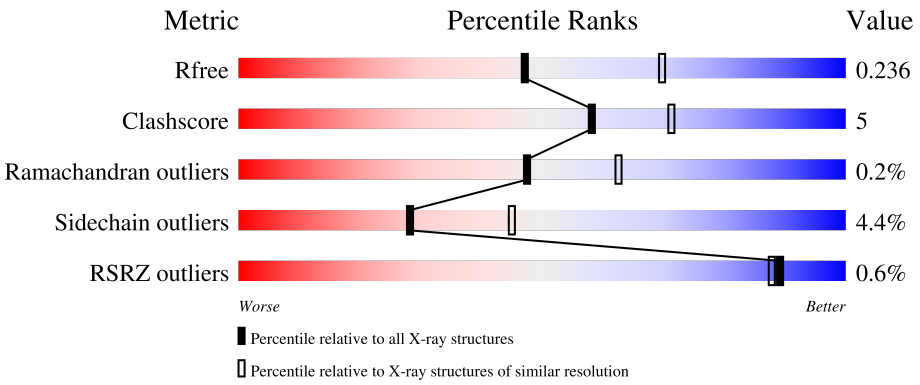
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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% • 18%
1	B	1032	71% 10% • 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
3	CD	A	1902	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14500 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.

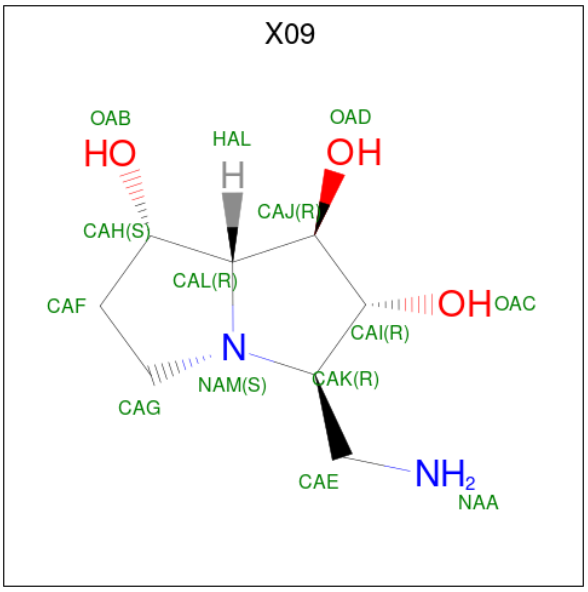
- Molecule 1 is a protein called EXO-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	851	6518	4095	1127	1279	17	15	1	1
1	B	851	6512	4090	1126	1279	17	9	0	1

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-AUSTRALINE (three-letter code: X09) (formula: $C_8H_{16}N_2O_3$).



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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	2	2	2	0	0
3	B	1	1	1	0	0

- Molecule 4 is water.

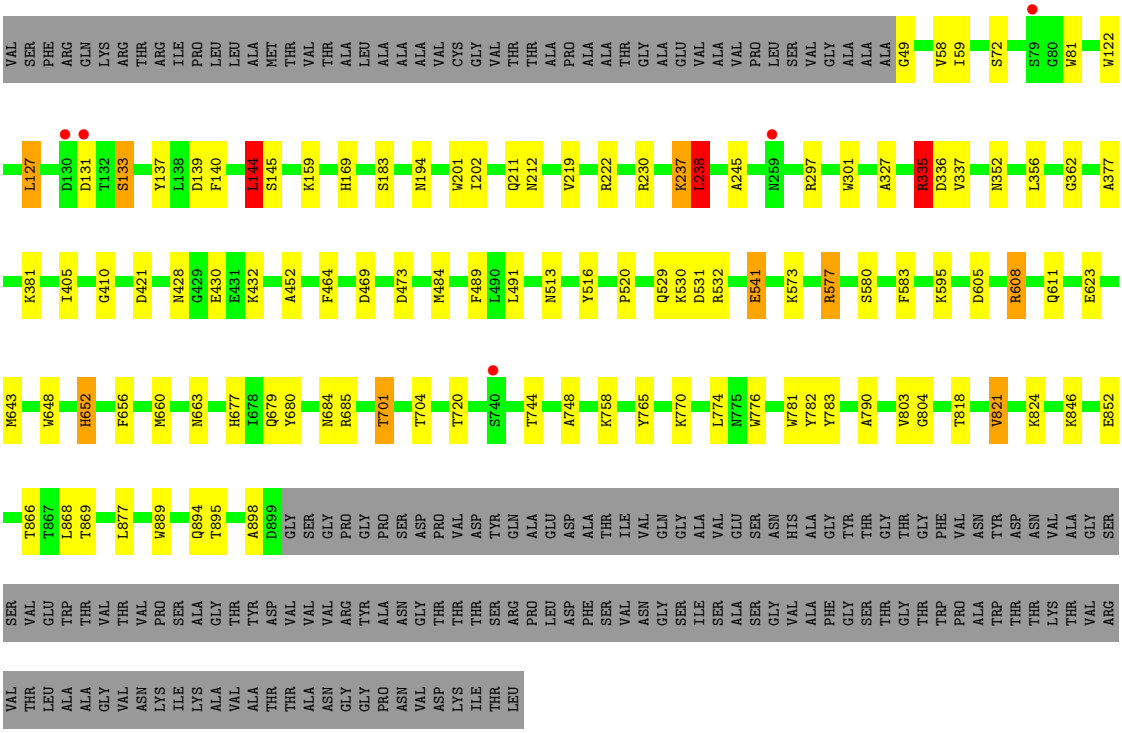
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	733	733	733	0	0
4	B	708	708	708	0	0

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.

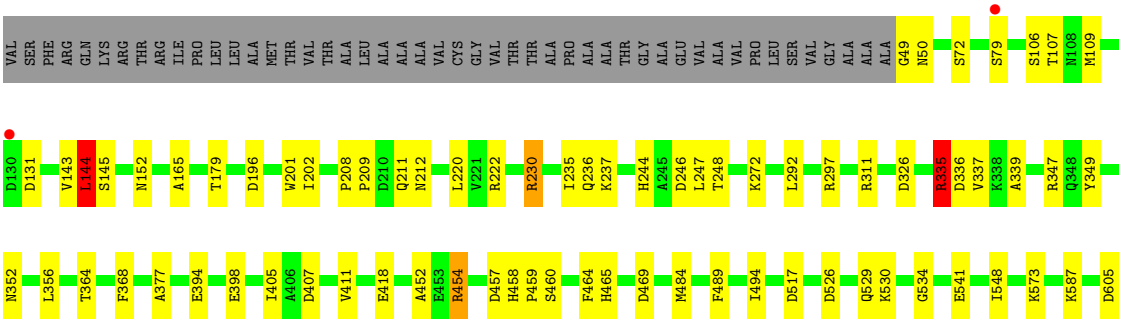
• Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

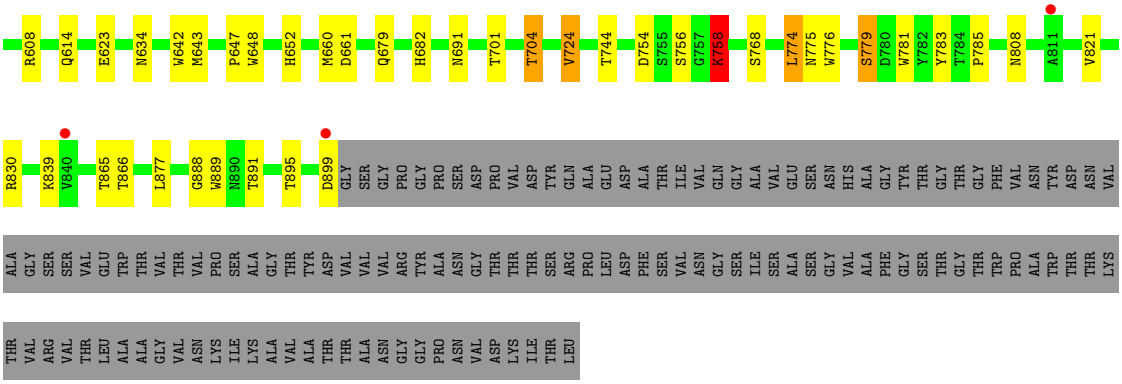
Chain A: 72% 9% • 18%



• Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain B: 71% 10% • 18%




R608
Q614
E623
N634
W642
M643
P647
W648
H652
M660
D661
Q679
H682
N691
T701
T704
V724
T744
D754
S755
S756
G757
K758
S768
L774
N775
W776
S779
D780
W781
Y782
Y783
T784
P785
N808
A811
V821
R830
K839
V840
T865
T866
L877
G888
W889
N890
T891
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	86.75Å 121.95Å 92.05Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.40) 96.7 (19.99-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.176 , 0.240 0.175 , 0.236	Depositor DCC
R_{free} test set	3652 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14500	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: X09, 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	0.61	4/6684 (0.1%)	0.74	10/9119 (0.1%)
1	B	0.84	4/6675 (0.1%)	0.77	10/9108 (0.1%)
All	All	0.73	8/13359 (0.1%)	0.75	20/18227 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	ARG	CD-NE	-34.45	0.87	1.46
1	B	530	LYS	CD-CE	24.63	2.12	1.51
1	B	758	LYS	CD-CE	-22.07	0.96	1.51
1	B	573	LYS	CE-NZ	-16.59	1.07	1.49
1	A	127	LEU	CG-CD1	-15.65	0.94	1.51
1	A	432	LYS	CG-CD	-10.54	1.16	1.52
1	A	898	ALA	CA-CB	-9.59	1.32	1.52
1	A	127	LEU	CG-CD2	7.76	1.80	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	297	ARG	CG-CD-NE	23.39	160.91	111.80
1	A	127	LEU	CB-CG-CD1	23.14	150.35	111.00
1	B	297	ARG	CD-NE-CZ	14.76	144.27	123.60
1	A	127	LEU	CB-CG-CD2	-14.21	86.84	111.00
1	B	573	LYS	CD-CE-NZ	11.70	138.61	111.70
1	B	530	LYS	CG-CD-CE	-10.81	79.48	111.90
1	A	573	LYS	CB-CG-CD	-9.18	87.75	111.60
1	A	898	ALA	N-CA-CB	7.06	119.99	110.10
1	A	144	LEU	CA-CB-CG	7.00	131.39	115.30
1	A	335	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	335	ARG	NE-CZ-NH2	-6.37	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	758	LYS	CD-CE-NZ	-6.19	97.46	111.70
1	B	144	LEU	CA-CB-CG	6.09	129.30	115.30
1	B	454	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	573	LYS	CG-CD-CE	-5.77	94.60	111.90
1	A	230	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	238	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	774	LEU	CA-CB-CG	-5.27	103.19	115.30
1	B	230	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	335	ARG	NE-CZ-NH1	5.19	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

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	6518	0	6298	58	0
1	B	6512	0	6285	63	2
2	A	13	0	16	5	0
2	B	13	0	16	4	0
3	A	2	0	0	0	2
3	B	1	0	0	0	0
4	A	733	0	0	2	0
4	B	708	0	0	11	0
All	All	14500	0	12615	123	2

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 (123) 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	1.68	1.06
1:B:201:TRP:HE1	1:B:212:ASN:HD21	1.04	0.98
1:A:201:TRP:HE1	1:A:212:ASN:HD21	1.10	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:CA	4:B:2149:HOH:O	2.14	0.95
1:B:109:MET:CE	1:B:368:PHE:CE1	2.50	0.94
1:B:109:MET:HE1	1:B:368:PHE:CE1	2.07	0.90
1:B:109:MET:HE1	1:B:368:PHE:HE1	1.36	0.89
1:A:577:ARG:HG2	1:A:583:PHE:O	1.74	0.88
1:A:297:ARG:HG3	4:B:2010:HOH:O	1.74	0.87
1:B:336:ASP:H	1:B:352:ASN:ND2	1.77	0.82
1:B:109:MET:HE2	1:B:208:PRO:HA	1.61	0.82
1:B:469:ASP:OD2	2:B:1900:X09:HAE1	1.81	0.81
1:A:608:ARG:HG3	1:A:889:TRP:CZ3	2.19	0.77
1:B:109:MET:HE2	1:B:209:PRO:HD3	1.65	0.77
1:B:109:MET:HE3	1:B:368:PHE:CE1	2.21	0.76
2:B:1900:X09:HAG1	4:B:2415:HOH:O	1.88	0.73
1:B:776:TRP:O	1:B:779:SER:HB2	1.89	0.72
1:B:548:ILE:H	1:B:614:GLN:HE22	1.38	0.72
1:B:336:ASP:H	1:B:352:ASN:HD22	1.37	0.70
1:A:541:GLU:OE1	2:A:1900:X09:HAE2	1.92	0.69
1:A:139:ASP:OD2	1:A:222:ARG:NH1	2.28	0.67
1:A:131:ASP:OD2	1:A:133:SER:HB2	1.95	0.65
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.62	0.65
1:A:201:TRP:HE1	1:A:212:ASN:ND2	1.89	0.64
1:B:311:ARG:HD2	1:B:407:ASP:HB3	1.79	0.64
1:A:469:ASP:OD1	2:A:1900:X09:HAE1	1.98	0.64
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.63	0.63
1:A:803:VAL:O	1:A:894:GLN:NE2	2.30	0.63
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.86	0.62
1:B:548:ILE:H	1:B:614:GLN:NE2	1.97	0.62
1:B:349:TYR:OH	1:B:494:ILE:HD11	1.99	0.62
1:A:336:ASP:H	1:A:352:ASN:ND2	1.98	0.61
1:B:754:ASP:OD2	1:B:758:LYS:HG2	2.00	0.61
1:A:680:TYR:OH	1:A:685:ARG:HG2	2.02	0.60
1:A:577:ARG:HD2	1:A:652:HIS:CG	2.37	0.59
1:B:605:ASP:HA	1:B:608:ARG:HD3	1.85	0.57
1:B:398:GLU:O	1:B:454:ARG:NH2	2.37	0.57
1:B:704:THR:HG23	4:B:2572:HOH:O	2.06	0.56
1:A:577:ARG:HD2	1:A:652:HIS:ND1	2.19	0.56
1:B:899:ASP:N	4:B:2707:HOH:O	2.40	0.55
1:A:623:GLU:HG2	1:A:679:GLN:NE2	2.23	0.54
1:B:311:ARG:HD3	4:B:2360:HOH:O	2.07	0.54
1:A:237:LYS:HE3	1:A:238:LEU:H	1.73	0.53
2:A:1900:X09:HAG1	4:A:2437:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:ARG:HG3	1:B:889:TRP:CZ3	2.43	0.52
1:B:605:ASP:O	1:B:608:ARG:HG2	2.11	0.50
1:B:682:HIS:HE1	4:B:2524:HOH:O	1.94	0.50
1:B:704:THR:CG2	4:B:2572:HOH:O	2.59	0.49
1:A:139:ASP:HA	1:A:169:HIS:O	2.12	0.49
1:A:464:PHE:HB3	1:A:484:MET:HE1	1.95	0.48
1:B:364:THR:HG21	1:B:647:PRO:HD3	1.93	0.48
1:B:642:TRP:CD2	1:B:643:MET:HG2	2.48	0.48
1:A:677:HIS:CD2	1:A:679:GLN:HE21	2.31	0.48
1:A:377:ALA:HA	1:A:405:ILE:HG21	1.95	0.47
1:A:194:ASN:HD22	1:A:421:ASP:HA	1.79	0.47
1:A:770:LYS:O	1:A:790:ALA:HA	2.14	0.47
1:B:526:ASP:O	1:B:534:GLY:HA3	2.14	0.47
1:A:137:TYR:HB2	1:A:222:ARG:HB2	1.95	0.47
1:A:701:THR:HB	1:A:720:THR:HA	1.95	0.47
1:B:623:GLU:HG2	1:B:679:GLN:OE1	2.14	0.47
1:A:140:PHE:HB3	1:A:219:VAL:HA	1.97	0.47
1:A:58:VAL:HB	1:A:81:TRP:HB3	1.96	0.47
1:A:821:VAL:HG13	1:A:868:LEU:HB2	1.97	0.47
1:B:246:ASP:HB3	1:B:292:LEU:HD11	1.96	0.47
1:B:452:ALA:HB1	1:B:489:PHE:HB2	1.97	0.47
1:A:362:GLY:O	1:A:643:MET:HB3	2.15	0.47
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.97	0.46
1:B:109:MET:CE	1:B:209:PRO:HD3	2.41	0.46
1:B:691:ASN:HB3	1:B:724:VAL:HG22	1.97	0.46
1:A:144:LEU:HA	1:A:145:SER:HA	1.68	0.46
1:A:541:GLU:CD	2:A:1900:X09:HAE2	2.36	0.45
1:B:411:VAL:O	1:B:460:SER:HB2	2.17	0.45
1:A:529:GLN:HG3	1:A:776:TRP:CD2	2.51	0.45
1:B:394:GLU:OE2	2:B:1900:X09:NAA	2.50	0.45
1:B:196:ASP:HB3	4:B:2104:HOH:O	2.17	0.45
1:B:144:LEU:HD22	1:B:165:ALA:HB2	1.99	0.45
1:B:144:LEU:HD22	1:B:165:ALA:CB	2.47	0.44
1:B:661:ASP:OD1	1:B:839:LYS:NZ	2.49	0.44
1:A:49:GLY:HA2	1:A:327:ALA:H	1.83	0.44
1:A:532:ARG:HA	1:A:532:ARG:HD3	1.75	0.44
1:A:301:TRP:CZ2	1:A:410:GLY:HA2	2.52	0.44
1:A:748:ALA:HB3	1:A:765:TYR:HB2	2.00	0.43
1:A:781:TRP:CE3	1:A:782:TYR:HB3	2.54	0.43
1:A:677:HIS:HD2	1:A:679:GLN:HE21	1.67	0.43
1:B:394:GLU:HG2	1:B:418:GLU:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:THR:O	1:B:768:SER:HA	2.18	0.43
1:A:237:LYS:O	1:A:245:ALA:HA	2.18	0.43
1:B:775:ASN:HB3	1:B:785:PRO:HG2	2.01	0.42
1:A:381:LYS:HB3	1:A:852:GLU:OE2	2.19	0.42
1:A:818:THR:HG23	1:A:869:THR:HG23	2.01	0.42
1:B:72:SER:O	1:B:152:ASN:HA	2.20	0.42
1:B:144:LEU:HA	1:B:145:SER:HA	1.62	0.42
1:A:337:VAL:CG1	1:A:491:LEU:HD23	2.49	0.42
1:A:513:ASN:HB3	1:A:531:ASP:O	2.19	0.42
1:B:220:LEU:CD1	1:B:222:ARG:NH1	2.82	0.42
1:A:577:ARG:HD2	1:A:652:HIS:CB	2.49	0.42
1:A:605:ASP:HA	1:A:608:ARG:HD3	2.01	0.42
1:B:49:GLY:HA2	1:B:326:ASP:HA	2.02	0.42
1:B:220:LEU:HD13	1:B:222:ARG:NH1	2.35	0.42
1:B:339:ALA:HB1	1:B:347:ARG:HD2	2.01	0.42
1:A:656:PHE:CE1	1:A:660:MET:HE1	2.54	0.42
1:B:888:GLY:HA3	1:B:891:THR:OG1	2.19	0.42
1:B:235:ILE:HB	1:B:248:THR:HB	2.02	0.42
1:B:465:HIS:HD2	4:B:2364:HOH:O	2.03	0.42
1:B:529:GLN:HG3	1:B:776:TRP:CE3	2.54	0.42
1:A:473:ASP:OD1	1:A:473:ASP:C	2.59	0.41
1:A:577:ARG:CD	1:A:652:HIS:HB3	2.50	0.41
1:B:457:ASP:OD2	4:B:2411:HOH:O	2.22	0.41
1:B:781:TRP:HZ3	2:B:1900:X09:HAF1	1.85	0.41
1:A:59:ILE:HA	1:A:122:TRP:O	2.20	0.41
1:A:516:TYR:CE2	2:A:1900:X09:HAF2	2.56	0.41
1:A:804:GLY:HA3	1:A:824:LYS:O	2.22	0.40
1:B:377:ALA:HA	1:B:405:ILE:HG21	2.03	0.40
1:B:464:PHE:HB3	1:B:484:MET:HE1	2.03	0.40
1:A:72:SER:O	1:A:183:SER:HB2	2.21	0.40
1:A:520:PRO:HD2	1:A:774:LEU:HD21	2.02	0.40
1:A:684:ASN:O	1:A:685:ARG:HB2	2.22	0.40
1:B:109:MET:CE	1:B:368:PHE:CZ	3.03	0.40
1:A:337:VAL:HG11	1:A:491:LEU:CD2	2.50	0.40
1:A:530[A]:LYS:HG2	4:A:2489:HOH:O	2.21	0.40
1:A:611:GLN:OE1	1:A:663:ASN:HB2	2.21	0.40
1:B:106:SER:OG	1:B:107:THR:N	2.55	0.40
1:B:458:HIS:HA	1:B:459:PRO:HD2	1.84	0.40

All (2) 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:B:246:ASP:OD1	3:A:1902:CD:CD[2_557]	1.94	0.26
1:B:244:HIS:NE2	3:A:1902:CD:CD[2_557]	2.10	0.10

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	850/1032 (82%)	821 (97%)	27 (3%)	2 (0%)	47	62
1	B	849/1032 (82%)	819 (96%)	28 (3%)	2 (0%)	47	62
All	All	1699/2064 (82%)	1640 (96%)	55 (3%)	4 (0%)	47	62

All (4) Ramachandran outliers are listed below:

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

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	700/834 (84%)	674 (96%)	26 (4%)	34	53
1	B	699/834 (84%)	664 (95%)	35 (5%)	24	40
All	All	1399/1668 (84%)	1338 (96%)	61 (4%)	28	45

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	133	SER
1	A	144	LEU
1	A	159	LYS
1	A	211	GLN
1	A	237	LYS
1	A	238	LEU
1	A	335	ARG
1	A	356	LEU
1	A	428	ASN
1	A	430	GLU
1	A	577	ARG
1	A	580	SER
1	A	595	LYS
1	A	608	ARG
1	A	648	TRP
1	A	652	HIS
1	A	701	THR
1	A	704	THR
1	A	744	THR
1	A	783	TYR
1	A	821	VAL
1	A	846	LYS
1	A	866	THR
1	A	877	LEU
1	A	895	THR
1	B	50	ASN
1	B	79	SER
1	B	131	ASP
1	B	143	VAL
1	B	144	LEU
1	B	211	GLN
1	B	230	ARG
1	B	236	GLN
1	B	237	LYS
1	B	247	LEU
1	B	272	LYS
1	B	335	ARG
1	B	337	VAL
1	B	356	LEU
1	B	517	ASP
1	B	587	LYS

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Mol	Chain	Res	Type
1	B	634	ASN
1	B	648	TRP
1	B	652	HIS
1	B	660	MET
1	B	701	THR
1	B	704	THR
1	B	724	VAL
1	B	756	SER
1	B	758	LYS
1	B	774	LEU
1	B	779	SER
1	B	783	TYR
1	B	808	ASN
1	B	821	VAL
1	B	830	ARG
1	B	865	THR
1	B	866	THR
1	B	877	LEU
1	B	895	THR

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

Mol	Chain	Res	Type
1	A	194	ASN
1	A	211	GLN
1	A	212	ASN
1	A	276	GLN
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	529	GLN
1	A	679	GLN
1	A	750	ASN
1	A	796	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

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Mol	Chain	Res	Type
1	B	614	GLN
1	B	682	HIS
1	B	750	ASN
1	B	796	ASN
1	B	808	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	X09	B	1900	-	13,14,14	0.59	0	18,21,21	2.00	5 (27%)
2	X09	A	1900	-	13,14,14	0.77	0	18,21,21	1.83	3 (16%)

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	X09	B	1900	-	-	0/0/31/31	0/2/2/2
2	X09	A	1900	-	-	0/0/31/31	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1900	X09	CAJ-CAI-CAK	-5.17	94.15	102.45
2	B	1900	X09	CAJ-CAI-CAK	-4.82	94.71	102.45
2	B	1900	X09	CAI-CAJ-CAL	-4.08	97.36	102.82
2	A	1900	X09	CAI-CAJ-CAL	-3.81	97.73	102.82
2	B	1900	X09	CAG-NAM-CAK	2.71	120.07	114.98
2	B	1900	X09	CAI-CAK-NAM	-2.61	100.59	104.58
2	B	1900	X09	CAF-CAH-CAL	-2.07	100.21	102.80
2	A	1900	X09	CAE-CAK-NAM	-2.04	107.59	112.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1900	X09	4	0
2	A	1900	X09	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	-0.41	5 (0%)	89	88	6, 16, 27, 40	7 (0%)
1	B	851/1032 (82%)	-0.45	5 (0%)	89	88	4, 15, 26, 37	4 (0%)
All	All	1702/2064 (82%)	-0.43	10 (0%)	89	88	4, 15, 26, 40	11 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ASP	3.9
1	A	130	ASP	3.8
1	B	899	ASP	2.6
1	B	840	VAL	2.6
1	A	259	ASN	2.5
1	A	131	ASP	2.4
1	A	740	SER	2.4
1	B	79	SER	2.3
1	B	811	ALA	2.1
1	A	79	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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, 95th 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	X09	A	1900	13/13	0.93	0.13	13,16,17,19	0
2	X09	B	1900	13/13	0.95	0.12	12,14,15,15	0
3	CD	B	1901	1/1	0.98	0.22	66,66,66,66	0
3	CD	A	1902	1/1	1.00	0.03	9,9,9,9	0
3	CD	A	1901	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.