



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:46 AM UTC

PDB ID : 2X05 / pdb_00002x05
Title : Inhibition of the exo-beta-D-glucosaminidase CsxA by a glucosamine- configured castanospermine and an amino-australine analogue
Authors : Pluvinae, B.; Ghinet, M.G.; Brzezinski, R.; Boraston, A.B.; Stubbs, K.A.
Deposited on : 2009-12-05
Resolution : 2.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

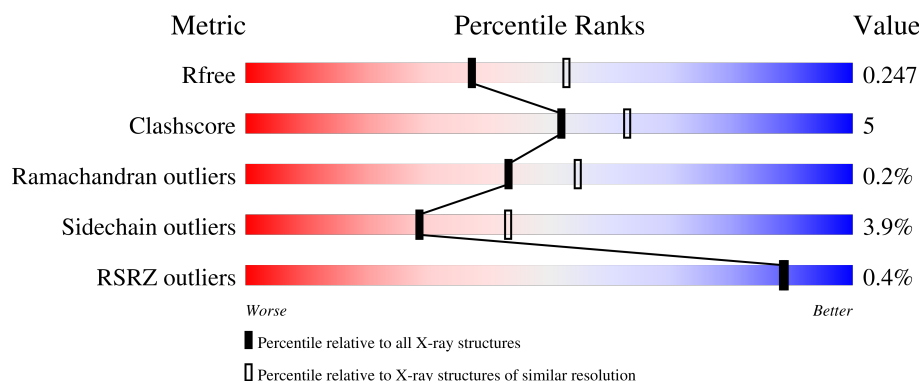
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	
1	B	1032	

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 14302 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.

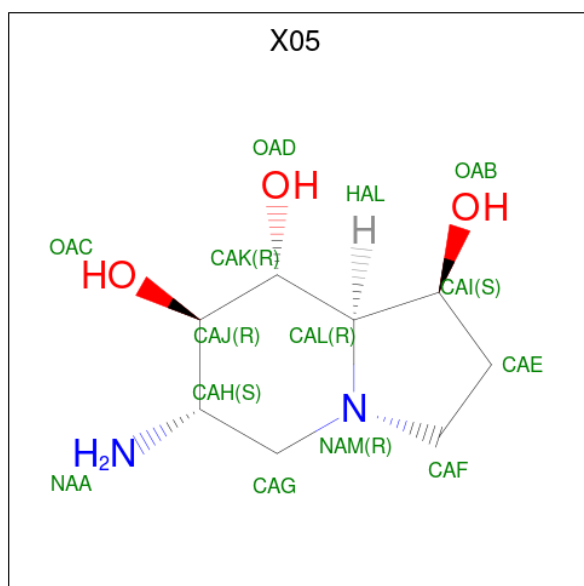
- Molecule 1 is a protein called EXO-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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 (CCD ID: X05) (formula: $C_8H_{16}N_2O_3$).



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 (CCD ID: CD) (formula: Cd).

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

- 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		

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.

[illegible]

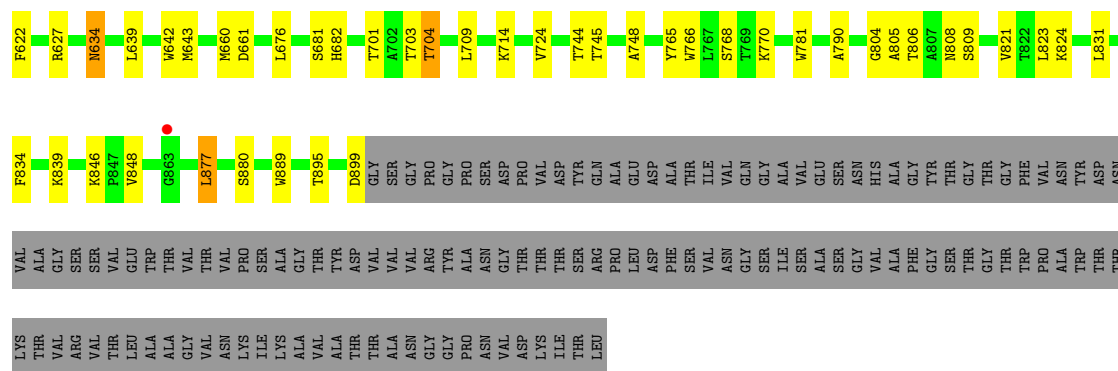
Chain B:

72% 10% 17%

Sequence logo for Chain B. The y-axis represents information content in bits. The x-axis represents positions 1 to 300. A color scale at the top indicates conservation levels: green (72%), yellow (10%), and red (17%).

Key residues (positions and amino acids):

- Position 1: VAL
- Position 2: SER
- Position 3: PHE
- Position 4: ARG
- Position 5: GLN
- Position 6: LYS
- Position 7: ARG
- Position 8: THR
- Position 9: ARG
- Position 10: ILE
- Position 11: PRO
- Position 12: LEU
- Position 13: LEU
- Position 14: MET
- Position 15: ALA
- Position 16: THR
- Position 17: VAL
- Position 18: THR
- Position 19: ALA
- Position 20: LEU
- Position 21: ALA
- Position 22: ALA
- Position 23: VAL
- Position 24: CYS
- Position 25: GLY
- Position 26: VAL
- Position 27: THR
- Position 28: THR
- Position 29: ALA
- Position 30: PRO
- Position 31: ALA
- Position 32: ALA
- Position 33: THR
- Position 34: GLY
- Position 35: ALA
- Position 36: GLU
- Position 37: VAL
- Position 38: ALA
- Position 39: VAL
- Position 40: PRO
- Position 41: LEU
- Position 42: SER
- Position 43: VAL
- Position 44: GLY
- Position 45: ALA
- Position 46: ALA
- Position 47: A48
- Position 48: G49
- Position 49: N50
- Position 50: Q60
- Position 51: S69
- Position 52: S72
- Position 53: S79
- Position 54: G80
- Position 55: Y81
- Position 56: S85
- Position 57: Y137
- Position 58: D139
- Position 59: V143
- Position 60: L144
- Position 61: S145
- Position 62: K148
- Position 63: A147
- Position 64: W150
- Position 65: H169
- Position 66: S183
- Position 67: K187
- Position 68: P193
- Position 69: W201
- Position 70: I202
- Position 71: A205
- Position 72: W212
- Position 73: R222
- Position 74: R230
- Position 75: Q236
- Position 76: K237
- Position 77: H244
- Position 78: A246
- Position 79: D246
- Position 80: L247
- Position 81: V253
- Position 82: L292
- Position 83: D296
- Position 84: W301
- Position 85: R311
- Position 86: T323
- Position 87: R336
- Position 88: D336
- Position 89: N352
- Position 90: T356



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	4188 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14302	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.68	1/6686 (0.0%)	0.90	4/9123 (0.0%)
1	B	0.68	0/6701	0.87	8/9143 (0.1%)
All	All	0.68	1/13387 (0.0%)	0.89	12/18266 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	8.43	1.77	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	GLU	CA-CB-CG	-8.82	96.45	114.10
1	B	805	ALA	N-CA-C	7.00	121.08	108.69
1	A	805	ALA	N-CA-C	6.85	120.07	108.90
1	B	634	ASN	CA-C-N	-5.67	114.13	119.85
1	B	634	ASN	C-N-CA	-5.67	114.13	119.85
1	A	119	VAL	CA-C-N	-5.30	114.78	120.03
1	A	119	VAL	C-N-CA	-5.30	114.78	120.03
1	B	518	TYR	N-CA-C	5.25	117.92	110.10
1	B	147	ALA	N-CA-C	5.21	117.66	108.75
1	B	831	LEU	N-CA-C	5.14	116.13	109.65
1	B	494	ILE	CA-C-N	5.11	124.72	119.05
1	B	494	ILE	C-N-CA	5.11	124.72	119.05

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	6520	0	6295	69	0
1	B	6532	0	6312	61	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	8	0
4	B	601	0	0	9	0
All	All	14302	0	12639	130	3

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 (130) 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	1.03	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:201:TRP:NE1	1:A:212:ASN:HD21	1.69	0.89
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:201:TRP:NE1	1:B:212:ASN:HD21	1.77	0.82
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:187:LYS:NZ	4:B:2113:HOH:O	2.10	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:201:TRP:O	1:B:202:ILE:C	2.51	0.53
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:804:GLY:O	1:B:823:LEU:HA	2.14	0.47
1:A:50:ASN:HB3	1:A:223:ARG:HB2	1.97	0.47
1:A:99:LYS:NZ	4:A:2037:HOH:O	2.39	0.47
1:A:687:VAL:HG21	1:A:704:THR:HG21	1.97	0.47
1:B:704:THR:HG22	4:B:2485:HOH:O	2.14	0.47
1:A:54:ILE:HG21	1:A:125:THR:HG21	1.98	0.46
1:B:526:ASP:O	1:B:534:GLY:HA3	2.15	0.46
1:A:781:TRP:HZ3	2:A:1900:X05:HAE1	1.81	0.46
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.97	0.46
1:B:781:TRP:CZ3	2:B:1900:X05:HAE1	2.51	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:744:THR:O	1:B:768:SER:HA	2.16	0.45
1:B:848:VAL:HG21	1:B:877:LEU:CD1	2.46	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:464:PHE:HB3	1:B:484:MET:HE1	1.99	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:107:THR:O	1:A:108:ASN:C	2.61	0.44
1:A:338:LYS:HD2	4:A:2259:HOH:O	2.17	0.44
1:B:301:TRP:CZ2	1:B:410:GLY:HA2	2.53	0.44
1:B:379:LYS:HG2	1:B:660[A]:MET:HE1	1.99	0.44
1:B:516:TYR:CZ	2:B:1900:X05:HAF2	2.52	0.44
1:A:781:TRP:CD1	1:A:781:TRP:H	2.35	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:A:448:MET:SD	1:A:484:MET:HE3	2.58	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:660[A]:MET:HA	1:B:660[A]:MET:HE2	2.00	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:252:ASP:HA	1:A:286:LYS:O	2.21	0.41
1:A:701:THR:HA	1:A:719:LYS:O	2.20	0.41
1:B:703:THR:HG22	4:B:2522:HOH:O	2.21	0.41
1:A:700:LEU:HD23	1:A:754:ASP:HA	2.03	0.41
1:B:60:GLN:HB2	1:B:81:TRP:CD2	2.55	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:280:LEU:HD21	1:A:286:LYS:HB2	2.01	0.40
1:A:774:LEU:HD13	1:A:776:TRP:CZ2	2.56	0.40
1:A:547:ASP:H	1:A:652:HIS:HA	1.87	0.40
1:A:678:ILE:HB	1:A:752:LEU:HB2	2.03	0.40
1:B:144:LEU:HA	1:B:145:SER:HA	1.68	0.40
1:A:465:HIS:HD2	4:A:2343:HOH:O	2.04	0.40
1:B:69:SER:HA	1:B:150:TRP:CZ3	2.55	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	Interatomic distance (Å)	Clash overlap (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%)	48	60
1	B	853/1032 (83%)	817 (96%)	33 (4%)	3 (0%)	30	38
All	All	1704/2064 (83%)	1641 (96%)	59 (4%)	4 (0%)	43	55

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%)	671 (96%)	29 (4%)	27	41
1	B	702/834 (84%)	676 (96%)	26 (4%)	30	45
All	All	1402/1668 (84%)	1347 (96%)	55 (4%)	28	43

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	131	ASP

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Mol	Chain	Res	Type
1	A	133	SER
1	A	144	LEU
1	A	237	LYS
1	A	238	LEU
1	A	272	LYS
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	577	ARG
1	A	586	LEU
1	A	608	ARG
1	A	676	LEU
1	A	685	ARG
1	A	701	THR
1	A	704	THR
1	A	724	VAL
1	A	780	ASP
1	A	806	THR
1	A	830	ARG
1	A	877	LEU
1	A	887	SER
1	A	895	THR
1	B	79	SER
1	B	85	SER
1	B	143	VAL
1	B	144	LEU
1	B	187	LYS
1	B	230	ARG
1	B	236	GLN
1	B	237	LYS
1	B	247	LEU
1	B	253	VAL
1	B	323	THR
1	B	356	LEU
1	B	432	LYS
1	B	539	ASN
1	B	587	LYS

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Mol	Chain	Res	Type
1	B	608	ARG
1	B	634	ASN
1	B	676	LEU
1	B	701	THR
1	B	704	THR
1	B	724	VAL
1	B	806	THR
1	B	821	VAL
1	B	846	LYS
1	B	877	LEU
1	B	895	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	96	GLN
1	A	211	GLN
1	A	212	ASN
1	A	262	GLN
1	A	276	GLN
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	539	ASN
1	A	679	GLN
1	A	682	HIS
1	A	750	ASN
1	A	796	ASN
1	B	128	ASN
1	B	212	ASN
1	B	244	HIS
1	B	276	GLN
1	B	299	ASN
1	B	352	ASN
1	B	385	ASN
1	B	465	HIS
1	B	478	GLN
1	B	614	GLN
1	B	654	GLN
1	B	682	HIS
1	B	750	ASN

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Mol	Chain	Res	Type
1	B	796	ASN
1	B	808	ASN
1	B	894	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.21	1 (7%)	15,21,21	1.07	1 (6%)
2	X05	B	1900	-	14,14,14	0.95	0	15,21,21	1.08	1 (6%)

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	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	X05	B	1900	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1900	X05	CAI-CAL	-2.27	1.52	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1900	X05	CAG-NAM-CAL	2.61	115.22	110.62
2	A	1900	X05	CAE-CAI-CAL	-2.28	99.95	102.80

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	A	1900	X05	4	0
2	B	1900	X05	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	852/1032 (82%)	-0.22	3 (0%)	88 89	8, 18, 28, 47	2 (0%)
1	B	852/1032 (82%)	-0.23	3 (0%)	88 89	7, 18, 27, 42	3 (0%)
All	All	1704/2064 (82%)	-0.23	6 (0%)	88 89	7, 18, 28, 47	5 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	5.9
1	A	49	GLY	2.6
1	B	50	ASN	2.4
1	A	128	ASN	2.1
1	A	48	ALA	2.1
1	B	863	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	CD	B	1910	1/1	0.86	0.37	154,154,154,154	0
3	CD	B	1906	1/1	0.88	0.34	132,132,132,132	0
2	X05	A	1900	13/13	0.88	0.10	14,17,20,21	0
3	CD	A	1908	1/1	0.89	0.27	169,169,169,169	0
2	X05	B	1900	13/13	0.91	0.09	15,16,18,19	0
3	CD	A	1907	1/1	0.92	0.31	118,118,118,118	0
3	CD	B	1908	1/1	0.92	0.30	146,146,146,146	0
3	CD	A	1904	1/1	0.92	0.17	76,76,76,76	0
3	CD	B	1909	1/1	0.93	0.35	112,112,112,112	0
3	CD	B	1905	1/1	0.94	0.22	93,93,93,93	0
3	CD	B	1903	1/1	0.94	0.23	93,93,93,93	0
3	CD	B	1907	1/1	0.94	0.38	139,139,139,139	0
3	CD	A	1906	1/1	0.95	0.29	116,116,116,116	0
3	CD	B	1904	1/1	0.95	0.33	97,97,97,97	0
3	CD	B	1901	1/1	0.96	0.08	69,69,69,69	0
3	CD	A	1903	1/1	0.98	0.07	60,60,60,60	0
3	CD	B	1902	1/1	0.98	0.16	60,60,60,60	0
3	CD	A	1901	1/1	0.99	0.07	29,29,29,29	0
3	CD	A	1909	1/1	0.99	0.04	14,14,14,14	0
3	CD	A	1902	1/1	1.00	0.05	11,11,11,11	0
3	CD	A	1905	1/1	1.00	0.05	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.