



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:47 pm BST

PDB ID : 3ZJ7
Title : Crystal structure of strictosidine glucosidase in complex with inhibitor-1
Authors : Xia, L.; Lin, H.; Panjikar, S.; Ruppert, M.; Castiglia, A.; Rajendran, C.;
Wang, M.; Schuebel, H.; Warzecha, H.; Jaeger, V.; Stoeckigt, J.
Deposited on : 2013-01-17
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

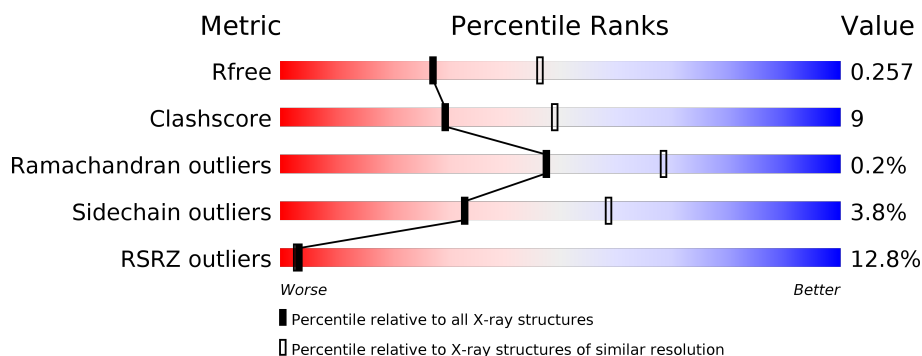
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	532	
1	B	532	

2 Entry composition [i](#)

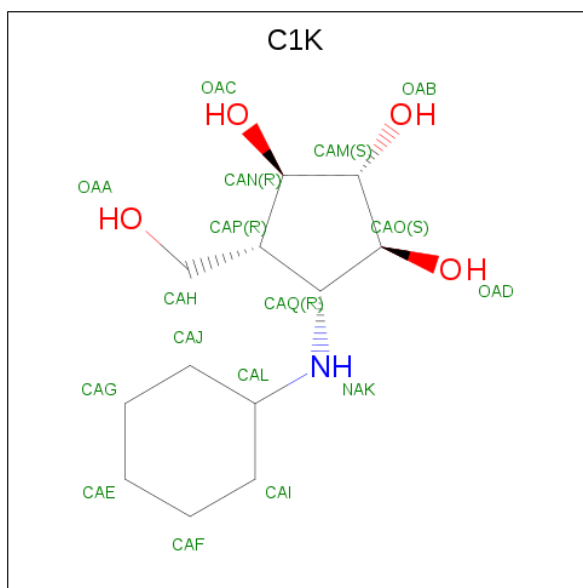
There are 3 unique types of molecules in this entry. The entry contains 7735 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STRICTOSIDINE-O-BETA-D-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3796	2444	632	705	15			
1	B	467	Total	C	N	O	S	0	0	0
			3796	2444	632	705	15			

- Molecule 2 is (1R,2S,3S,4R,5R)-4-(cyclohexylamino)-5-(hydroxymethyl)cyclopentane-1,2,3-triol (three-letter code: C1K) (formula: C₁₂H₂₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	12	1	4		
2	B	1	Total	C	N	O	0	0
			17	12	1	4		

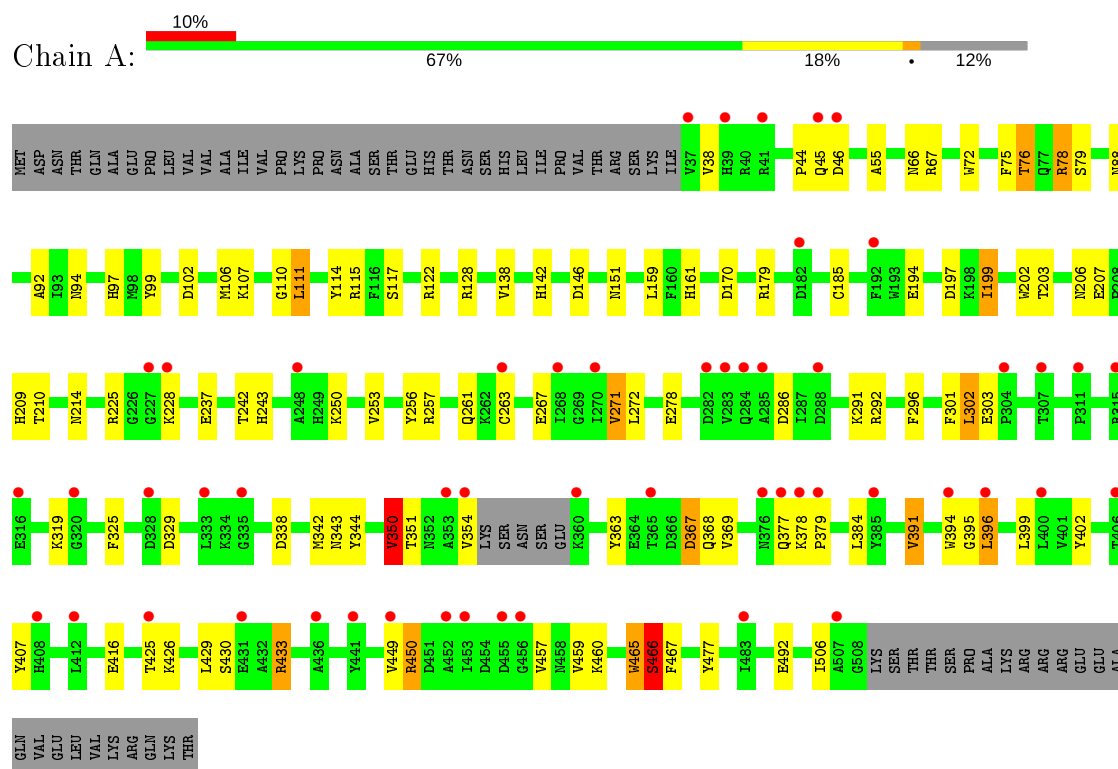
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total 56	O 56	0	0
3	B	53	Total 53	O 53	0	0

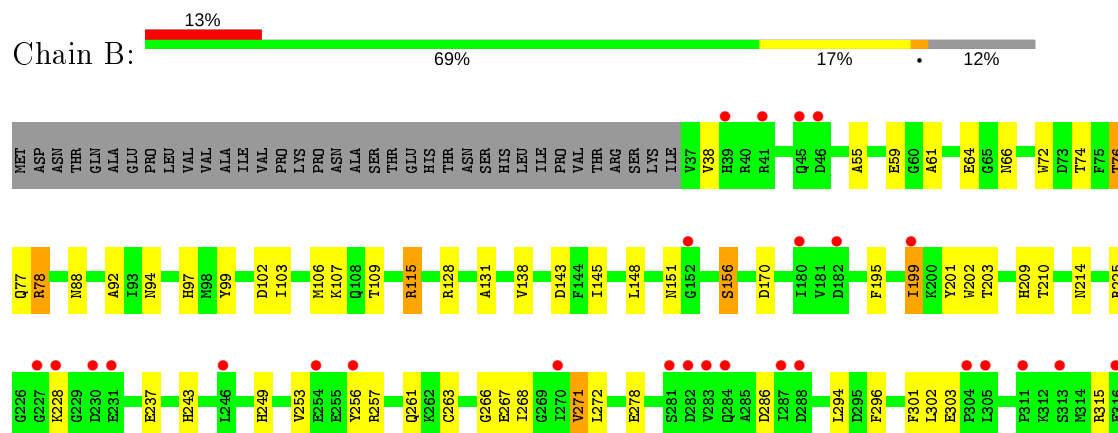
3 Residue-property plots [i](#)

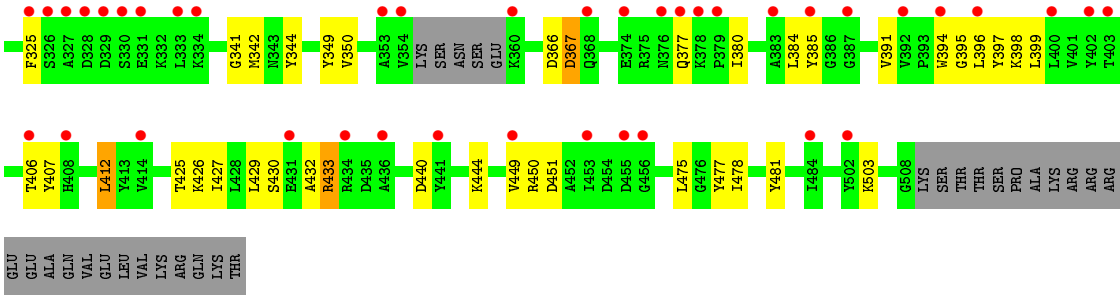
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: STRICTOSIDINE-O-BETA-D-GLUCOSIDASE



• Molecule 1: STRICTOSIDINE-O-BETA-D-GLUCOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.22Å 159.22Å 110.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.50 19.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.73-2.50) 97.6 (19.75-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.17 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.258 , 0.276 0.265 , 0.257	Depositor DCC
R_{free} test set	599 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7735	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: C1K

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	1.07	6/3908 (0.2%)	0.99	7/5292 (0.1%)
1	B	1.09	2/3908 (0.1%)	0.99	11/5292 (0.2%)
All	All	1.08	8/7816 (0.1%)	0.99	18/10584 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	VAL	CB-CG2	-6.78	1.38	1.52
1	A	350	VAL	CB-CG1	-6.70	1.38	1.52
1	B	350	VAL	CB-CG1	-6.18	1.39	1.52
1	A	114	TYR	CD1-CE1	5.52	1.47	1.39
1	A	99	TYR	CE1-CZ	5.35	1.45	1.38
1	B	78	ARG	CZ-NH1	-5.21	1.26	1.33
1	A	492	GLU	CD-OE1	5.15	1.31	1.25
1	A	185	CYS	CB-SG	-5.13	1.73	1.81

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	B	78	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	367	ASP	C-N-CA	-6.56	105.30	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	115	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	B	433	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	433	ARG	CB-CA-C	-5.69	99.01	110.40
1	B	451	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	412	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	450	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	B	450	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	A	146	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	433	ARG	CB-CA-C	-5.42	99.57	110.40
1	A	111	LEU	CB-CG-CD1	5.38	120.14	111.00
1	B	367	ASP	C-N-CA	-5.30	108.46	121.70
1	B	115	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	286	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	367	ASP	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	GLN	Peptide
1	A	465	TRP	Peptide

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	3796	0	3604	73	0
1	B	3796	0	3604	69	0
2	A	17	0	23	5	0
2	B	17	0	23	3	0
3	A	56	0	0	4	0
3	B	53	0	0	6	0
All	All	7735	0	7254	141	0

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 9.

All (141) 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)
2:A:1509:C1K:HAH1	2:A:1509:C1K:HAJ2	1.36	1.02
1:B:429:LEU:O	1:B:433:ARG:HG3	1.65	0.96
2:A:1509:C1K:HAH1	2:A:1509:C1K:CAJ	1.99	0.91
1:A:76:THR:HG21	1:A:88:ASN:HB2	1.54	0.87
2:B:1509:C1K:HAJ2	2:B:1509:C1K:HAH1	1.56	0.87
1:B:145:ILE:HD12	3:B:2035:HOH:O	1.75	0.85
1:B:195:PHE:HD1	3:B:2035:HOH:O	1.59	0.85
1:B:195:PHE:CD1	3:B:2035:HOH:O	2.33	0.82
1:B:76:THR:HG23	1:B:88:ASN:HB3	1.61	0.81
1:B:256:TYR:CE2	1:B:261:GLN:HB2	2.18	0.79
1:B:94:ASN:HD21	1:B:97:HIS:HD2	1.28	0.79
1:B:481:TYR:OH	3:B:2053:HOH:O	1.89	0.78
1:A:76:THR:CG2	1:A:88:ASN:HB2	2.15	0.77
1:A:76:THR:HG23	1:A:88:ASN:HB3	1.68	0.75
1:A:225:ARG:NH1	1:A:237:GLU:OE2	2.22	0.73
1:A:344:TYR:OH	1:A:395:GLY:HA3	1.88	0.73
1:A:94:ASN:HD21	1:A:97:HIS:HD2	1.36	0.72
1:A:203:THR:HG21	1:A:271:VAL:HG13	1.73	0.70
1:A:429:LEU:O	1:A:433:ARG:HG3	1.91	0.70
1:B:76:THR:HG21	1:B:88:ASN:HB2	1.72	0.69
1:B:61:ALA:HB1	1:B:64:GLU:HB2	1.74	0.69
1:A:203:THR:HG21	1:A:271:VAL:CG1	2.23	0.69
1:A:256:TYR:CE2	1:A:261:GLN:HB2	2.28	0.69
2:A:1509:C1K:HAJ2	2:A:1509:C1K:CAH	2.19	0.69
1:A:78:ARG:HD2	1:B:128:ARG:NH1	2.08	0.68
1:A:425:THR:O	1:A:426:LYS:HB2	1.94	0.68
1:A:76:THR:CG2	1:A:88:ASN:CB	2.71	0.67
1:B:266:GLY:O	1:B:267:GLU:HG2	1.95	0.67
1:B:203:THR:HG21	1:B:271:VAL:CG1	2.26	0.66
1:B:203:THR:HG21	1:B:271:VAL:HG13	1.76	0.66
1:A:72:TRP:O	1:A:76:THR:HB	1.96	0.64
1:B:94:ASN:HD21	1:B:97:HIS:CD2	2.13	0.64
1:A:76:THR:HG23	1:A:88:ASN:CB	2.27	0.63
1:B:427:ILE:HD11	1:B:432:ALA:HB2	1.80	0.63
2:B:1509:C1K:HAH1	2:B:1509:C1K:CAJ	2.27	0.63
1:B:76:THR:CG2	1:B:88:ASN:CB	2.77	0.62
1:B:72:TRP:O	1:B:76:THR:HB	1.99	0.62
1:A:465:TRP:CG	1:A:466:SER:N	2.64	0.62
1:B:76:THR:HG23	1:B:88:ASN:CB	2.29	0.61
1:A:46:ASP:OD2	1:A:460:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:O	1:A:257:ARG:HG3	2.01	0.60
1:A:384:LEU:HD11	1:A:391:VAL:HG12	1.83	0.60
1:B:243:HIS:CE1	1:B:325:PHE:CE1	2.90	0.60
1:B:76:THR:CG2	1:B:88:ASN:HB2	2.32	0.60
1:B:103:ILE:HG12	1:B:148:LEU:HD23	1.84	0.59
1:A:107:LYS:HD2	1:A:151:ASN:HD22	1.68	0.58
1:A:350:VAL:HG22	1:A:369:VAL:CG1	2.34	0.57
1:B:115:ARG:HG2	1:B:156:SER:OG	2.05	0.57
1:B:107:LYS:HD2	1:B:151:ASN:HD22	1.70	0.57
1:A:425:THR:O	1:A:426:LYS:CB	2.53	0.56
1:A:396:LEU:HD22	1:A:449:VAL:CG2	2.35	0.56
1:A:399:LEU:HG	1:A:399:LEU:O	2.05	0.56
1:B:210:THR:O	1:B:214:ASN:HB2	2.05	0.56
1:B:278:GLU:HG3	1:B:394:TRP:HH2	1.71	0.55
1:B:296:PHE:CG	1:B:367:ASP:HB3	2.41	0.55
1:A:207:GLU:OE1	2:A:1509:C1K:HAI1	2.07	0.55
1:A:44:PRO:C	1:A:46:ASP:H	2.10	0.55
1:A:75:PHE:O	1:A:79:SER:HB2	2.07	0.55
1:B:396:LEU:HD23	1:B:449:VAL:HG23	1.89	0.55
1:B:131:ALA:HB1	3:B:2033:HOH:O	2.07	0.54
1:A:303:GLU:OE1	1:A:407:TYR:HE1	1.90	0.54
1:A:350:VAL:HG22	1:A:369:VAL:HG11	1.89	0.54
1:B:425:THR:O	1:B:426:LYS:HB2	2.08	0.54
1:A:296:PHE:CG	1:A:367:ASP:HB3	2.44	0.53
1:A:242:THR:HG23	1:A:301:PHE:CE2	2.44	0.53
1:A:243:HIS:CE1	1:A:325:PHE:CE1	2.96	0.52
1:A:111:LEU:HD11	1:A:467:PHE:CE1	2.44	0.52
2:A:1509:C1K:HAH1	2:A:1509:C1K:CAL	2.29	0.51
1:A:278:GLU:HG3	1:A:394:TRP:HH2	1.73	0.51
1:B:74:THR:HG23	1:B:78:ARG:HD2	1.93	0.51
1:B:272:LEU:N	1:B:341:GLY:O	2.38	0.51
1:A:66:ASN:ND2	1:B:66:ASN:H	2.09	0.51
1:A:210:THR:O	1:A:214:ASN:HB2	2.12	0.50
1:B:249:HIS:O	1:B:253:VAL:HG23	2.12	0.49
1:A:66:ASN:HD21	1:B:66:ASN:H	1.61	0.49
1:B:366:ASP:C	1:B:367:ASP:O	2.50	0.48
1:B:92:ALA:HA	1:B:477:TYR:OH	2.13	0.48
1:A:102:ASP:O	1:A:106:MET:HG3	2.14	0.48
1:B:38:VAL:HG12	3:B:2001:HOH:O	2.13	0.48
1:B:399:LEU:O	1:B:399:LEU:HG	2.11	0.48
1:A:272:LEU:O	1:A:342:MET:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:NZ	1:A:402:TYR:OH	2.37	0.48
1:A:225:ARG:HH11	1:A:237:GLU:CD	2.17	0.48
1:B:303:GLU:OE1	1:B:407:TYR:HE1	1.97	0.48
1:B:384:LEU:HD11	1:B:391:VAL:HG12	1.96	0.48
1:A:237:GLU:HB2	3:A:2043:HOH:O	2.13	0.47
1:B:225:ARG:NH1	1:B:237:GLU:OE2	2.48	0.47
1:A:250:LYS:NZ	1:A:329:ASP:OD1	2.44	0.47
2:B:1509:C1K:CAL	2:B:1509:C1K:HAH1	2.46	0.46
1:A:170:ASP:CG	1:B:170:ASP:HB3	2.35	0.46
1:A:286:ASP:OD1	1:A:351:THR:OG1	2.06	0.45
1:B:396:LEU:CD2	1:B:449:VAL:HG23	2.46	0.45
1:A:199:ILE:HD11	1:A:202:TRP:CE2	2.52	0.45
1:A:396:LEU:HD22	1:A:449:VAL:HG23	1.98	0.45
1:A:292:ARG:HE	1:A:368:GLN:H	1.63	0.45
1:B:475:LEU:O	1:B:478:ILE:HG12	2.17	0.45
1:A:319:LYS:HG2	1:A:319:LYS:HZ2	1.67	0.45
1:A:396:LEU:HD22	1:A:449:VAL:HG22	1.99	0.45
1:B:156:SER:HB2	1:B:201:TYR:HB2	1.99	0.45
1:A:457:VAL:HG12	1:A:459:VAL:HG23	1.99	0.45
1:B:102:ASP:O	1:B:106:MET:HG3	2.17	0.45
1:A:225:ARG:HD3	1:A:237:GLU:OE1	2.17	0.44
1:B:243:HIS:CE1	1:B:325:PHE:CD1	3.06	0.44
1:A:197:ASP:CG	3:A:2039:HOH:O	2.56	0.44
1:A:92:ALA:HA	1:A:477:TYR:OH	2.17	0.44
1:B:202:TRP:O	1:B:268:ILE:HA	2.18	0.44
1:B:55:ALA:O	1:B:59:GLU:HB2	2.17	0.44
1:B:199:ILE:HD11	1:B:202:TRP:CD1	2.54	0.43
1:B:209:HIS:HB2	1:B:301:PHE:HE1	1.83	0.43
1:A:67:ARG:HB2	1:A:122:ARG:HG3	1.99	0.43
1:B:256:TYR:CD2	1:B:261:GLN:HB2	2.54	0.43
1:B:76:THR:HG22	1:B:77:GLN:HG3	2.00	0.43
1:A:128:ARG:HD3	3:A:2029:HOH:O	2.19	0.42
1:B:349:TYR:CE2	1:B:380:ILE:HB	2.55	0.42
1:A:450:ARG:HH11	1:A:450:ARG:HD3	1.68	0.42
1:A:363:TYR:C	1:A:363:TYR:CD1	2.93	0.42
1:A:66:ASN:H	1:B:66:ASN:ND2	2.17	0.42
1:A:110:GLY:O	1:A:506:ILE:HG21	2.19	0.42
1:A:267:GLU:OE1	1:A:338:ASP:HB3	2.19	0.42
1:B:253:VAL:O	1:B:257:ARG:HG3	2.20	0.42
1:B:344:TYR:OH	1:B:395:GLY:HA3	2.19	0.42
1:A:197:ASP:N	3:A:2039:HOH:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HD11	1:A:202:TRP:CD1	2.55	0.42
1:A:161:HIS:CE1	1:A:206:ASN:ND2	2.88	0.42
1:A:209:HIS:HB2	1:A:301:PHE:HE1	1.85	0.41
1:B:397:TYR:O	1:B:398:LYS:C	2.59	0.41
1:A:66:ASN:H	1:B:66:ASN:HD21	1.67	0.41
1:B:296:PHE:CD1	1:B:367:ASP:HB3	2.55	0.41
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.79	0.41
1:B:302:LEU:HA	1:B:302:LEU:HD12	1.55	0.41
1:B:396:LEU:HD21	1:B:449:VAL:CG2	2.51	0.41
1:A:142:HIS:CE1	1:A:194:GLU:O	2.74	0.41
1:A:343:ASN:CG	1:A:416:GLU:HB2	2.41	0.41
1:B:109:THR:O	1:B:503:LYS:HA	2.21	0.41
1:A:170:ASP:HB3	1:B:170:ASP:CG	2.41	0.40
1:B:440:ASP:OD2	1:B:444:LYS:HE2	2.21	0.40
1:B:425:THR:O	1:B:426:LYS:CB	2.67	0.40
1:A:170:ASP:HB3	1:B:170:ASP:HB3	2.02	0.40
1:A:378:LYS:HA	1:A:379:PRO:HD3	1.99	0.40
1:A:55:ALA:HB2	1:A:117:SER:O	2.22	0.40
1:B:99:TYR:OH	1:B:143:ASP:HB3	2.21	0.40

There are no symmetry-related clashes.

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	463/532 (87%)	436 (94%)	26 (6%)	1 (0%)	47	68
1	B	463/532 (87%)	433 (94%)	29 (6%)	1 (0%)	47	68
All	All	926/1064 (87%)	869 (94%)	55 (6%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	SER
1	B	385	TYR

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	396/456 (87%)	379 (96%)	17 (4%)	29	53
1	B	396/456 (87%)	383 (97%)	13 (3%)	38	64
All	All	792/912 (87%)	762 (96%)	30 (4%)	33	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	76	THR
1	A	138	VAL
1	A	159	LEU
1	A	179	ARG
1	A	199	ILE
1	A	228	LYS
1	A	263	CYS
1	A	271	VAL
1	A	302	LEU
1	A	350	VAL
1	A	354	VAL
1	A	377	GLN
1	A	391	VAL
1	A	396	LEU
1	A	430	SER
1	A	466	SER
1	B	76	THR
1	B	138	VAL
1	B	156	SER
1	B	199	ILE
1	B	228	LYS

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Mol	Chain	Res	Type
1	B	263	CYS
1	B	271	VAL
1	B	294	LEU
1	B	342	MET
1	B	377	GLN
1	B	406	THR
1	B	412	LEU
1	B	430	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	57	GLN
1	A	66	ASN
1	A	77	GLN
1	A	94	ASN
1	A	97	HIS
1	A	108	GLN
1	A	151	ASN
1	A	161	HIS
1	A	206	ASN
1	A	214	ASN
1	A	264	GLN
1	A	504	ASN
1	B	66	ASN
1	B	77	GLN
1	B	94	ASN
1	B	97	HIS
1	B	108	GLN
1	B	151	ASN
1	B	214	ASN
1	B	264	GLN
1	B	504	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	C1K	B	1509	-	18,18,18	1.60	4 (22%)	19,25,25	1.67	4 (21%)
2	C1K	A	1509	-	18,18,18	1.68	4 (22%)	19,25,25	1.09	1 (5%)

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	C1K	B	1509	-	-	3/6/34/34	0/2/2/2
2	C1K	A	1509	-	-	4/6/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1509	C1K	CAG-CAJ	3.39	1.62	1.53
2	B	1509	C1K	CAO-CAQ	3.17	1.59	1.53
2	A	1509	C1K	CAG-CAJ	3.06	1.61	1.53
2	A	1509	C1K	CAO-CAQ	3.02	1.59	1.53
2	B	1509	C1K	OAD-CAO	2.27	1.48	1.43
2	A	1509	C1K	CAE-CAF	2.24	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1509	C1K	OAD-CAO	2.18	1.48	1.43
2	B	1509	C1K	CAP-CAN	-2.18	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1509	C1K	CAP-CAN-CAM	-3.68	99.07	103.81
2	B	1509	C1K	CAJ-CAL-CAI	-3.51	104.74	110.82
2	A	1509	C1K	CAH-CAP-CAN	-3.07	106.20	114.31
2	B	1509	C1K	OAA-CAH-CAP	-2.98	104.41	111.29
2	B	1509	C1K	CAH-CAP-CAN	-2.92	106.59	114.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1509	C1K	OAA-CAH-CAP-CAQ
2	B	1509	C1K	OAA-CAH-CAP-CAN
2	A	1509	C1K	OAA-CAH-CAP-CAQ
2	A	1509	C1K	OAA-CAH-CAP-CAN
2	B	1509	C1K	CAI-CAL-NAK-CAQ
2	A	1509	C1K	CAI-CAL-NAK-CAQ
2	A	1509	C1K	CAJ-CAL-NAK-CAQ

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1509	C1K	3	0
2	A	1509	C1K	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 ⓘ

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, 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	467/532 (87%)	0.91	53 (11%) 5 4	35, 39, 45, 57	0
1	B	467/532 (87%)	0.99	67 (14%) 2 2	35, 39, 45, 55	0
All	All	934/1064 (87%)	0.95	120 (12%) 3 3	35, 39, 45, 57	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	VAL	6.4
1	A	283	VAL	5.6
1	A	408	HIS	5.2
1	B	408	HIS	5.1
1	B	376	ASN	5.1
1	A	45	GLN	4.8
1	B	377	GLN	4.7
1	B	328	ASP	4.6
1	B	406	THR	4.5
1	A	39	HIS	4.3
1	B	456	GLY	4.3
1	B	39	HIS	4.3
1	A	456	GLY	4.3
1	A	455	ASP	4.3
1	B	283	VAL	4.0
1	B	326	SER	4.0
1	B	228	LYS	3.8
1	B	304	PRO	3.8
1	A	354	VAL	3.8
1	A	353	ALA	3.7
1	A	379	PRO	3.6
1	B	387	GLY	3.5
1	A	406	THR	3.5
1	B	281	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	455	ASP	3.4
1	A	360	LYS	3.4
1	A	376	ASN	3.3
1	B	385	TYR	3.3
1	B	333	LEU	3.2
1	A	227	GLY	3.2
1	B	287	ILE	3.2
1	A	284	GLN	3.2
1	B	199	ILE	3.2
1	A	436	ALA	3.1
1	A	453	ILE	3.1
1	B	311	PRO	3.1
1	B	316	GLU	3.1
1	A	228	LYS	3.1
1	B	313	SER	3.0
1	B	330	SER	3.0
1	B	327	ALA	3.0
1	B	254	GLU	3.0
1	B	180	ILE	2.9
1	B	284	GLN	2.9
1	A	378	LYS	2.9
1	B	45	GLN	2.9
1	A	365	THR	2.9
1	A	311	PRO	2.9
1	B	396	LEU	2.9
1	A	316	GLU	2.8
1	A	377	GLN	2.8
1	B	383	ALA	2.8
1	B	374	GLU	2.8
1	B	400	LEU	2.8
1	A	263	CYS	2.8
1	B	246	LEU	2.8
1	B	394	TRP	2.7
1	A	449	VAL	2.7
1	A	333	LEU	2.7
1	B	379	PRO	2.7
1	A	315	ARG	2.7
1	B	449	VAL	2.7
1	B	378	LYS	2.7
1	B	325	PHE	2.7
1	B	46	ASP	2.7
1	A	385	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	46	ASP	2.7
1	A	394	TRP	2.6
1	A	400	LEU	2.6
1	B	231	GLU	2.6
1	B	434	ARG	2.6
1	A	431	GLU	2.6
1	A	307	THR	2.5
1	B	502	TYR	2.5
1	B	403	THR	2.5
1	B	305	LEU	2.5
1	B	270	ILE	2.5
1	A	268	ILE	2.5
1	A	441	TYR	2.4
1	B	414	VAL	2.4
1	A	288	ASP	2.4
1	A	304	PRO	2.4
1	B	431	GLU	2.4
1	B	282	ASP	2.4
1	A	452	ALA	2.4
1	B	353	ALA	2.4
1	B	402	TYR	2.3
1	B	152	GLY	2.3
1	B	41	ARG	2.3
1	B	227	GLY	2.3
1	B	441	TYR	2.3
1	B	329	ASP	2.3
1	A	396	LEU	2.3
1	B	331	GLU	2.3
1	A	41	ARG	2.2
1	A	483	ILE	2.2
1	A	507	ALA	2.2
1	B	436	ALA	2.2
1	A	425	THR	2.2
1	A	320	GLY	2.2
1	B	182	ASP	2.2
1	B	334	LYS	2.1
1	B	368	GLN	2.1
1	A	328	ASP	2.1
1	B	484	ILE	2.1
1	A	192	PHE	2.1
1	A	182	ASP	2.1
1	B	392	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	37	VAL	2.1
1	B	256	TYR	2.1
1	A	412	LEU	2.1
1	A	282	ASP	2.1
1	B	360	LYS	2.1
1	B	230	ASP	2.1
1	A	335	GLY	2.1
1	A	270	ILE	2.0
1	B	288	ASP	2.0
1	A	248	ALA	2.0
1	A	285	ALA	2.0
1	B	453	ILE	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 carbohydrates 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(\AA^2)	Q<0.9
2	C1K	B	1509	17/17	0.83	0.25	45,56,71,73	0
2	C1K	A	1509	17/17	0.83	0.23	50,57,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.