



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:25 pm BST

PDB ID : 3VNM
Title : Crystal structures of D-Psicose 3-epimerase with D-sorbose from *Clostridium cellulolyticum* H10
Authors : Chan, H.C.; Zhu, Y.; Hu, Y.; Ko, T.P.; Huang, C.H.; Ren, F.; Chen, C.C.; Guo, R.T.; Sun, Y.
Deposited on : 2012-01-17
Resolution : 2.12 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

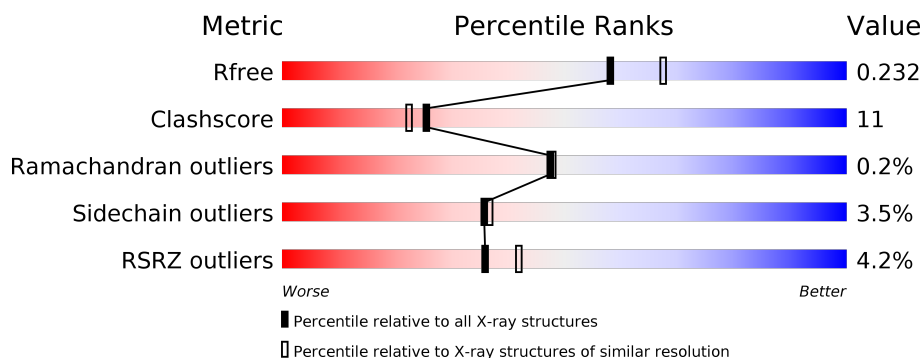
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	293	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	293	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	C	293	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>
1	D	293	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

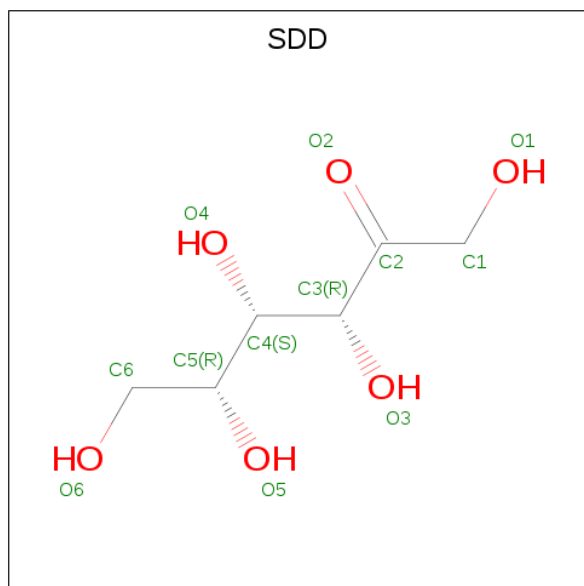
There are 4 unique types of molecules in this entry. The entry contains 9870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xylose isomerase domain protein TIM barrel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2292	1458	388	435	11			
1	B	290	Total	C	N	O	S	0	0	0
			2303	1465	391	436	11			
1	C	288	Total	C	N	O	S	0	0	0
			2287	1456	387	434	10			
1	D	290	Total	C	N	O	S	0	0	0
			2303	1465	391	436	11			

- Molecule 2 is D-sorbose (three-letter code: SDD) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mn	0	0
			3	3		
3	A	2	Total	Mn	0	0
			2	2		
3	D	1	Total	Mn	0	0
			1	1		
3	C	2	Total	Mn	0	0
			2	2		

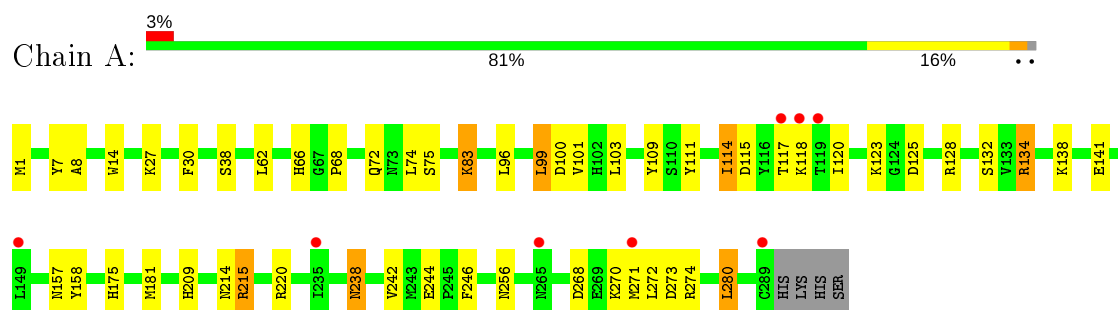
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	0
			213	213		
4	B	157	Total	O	0	0
			157	157		
4	C	123	Total	O	0	0
			123	123		
4	D	136	Total	O	0	0
			136	136		

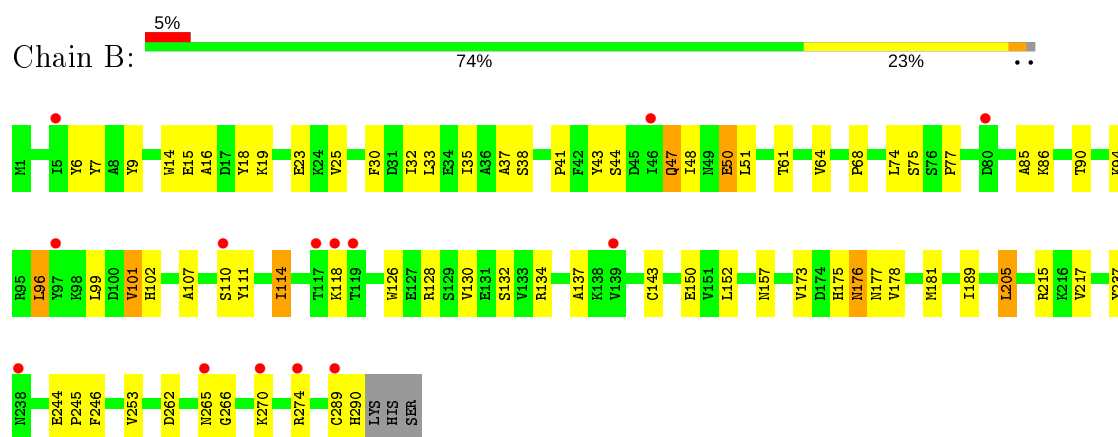
3 Residue-property plots [i](#)

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.

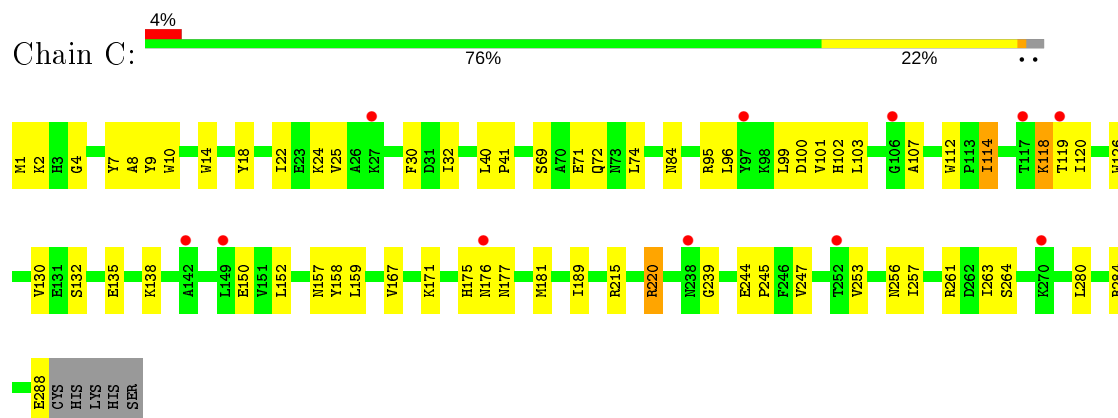
- Molecule 1: Xylose isomerase domain protein TIM barrel



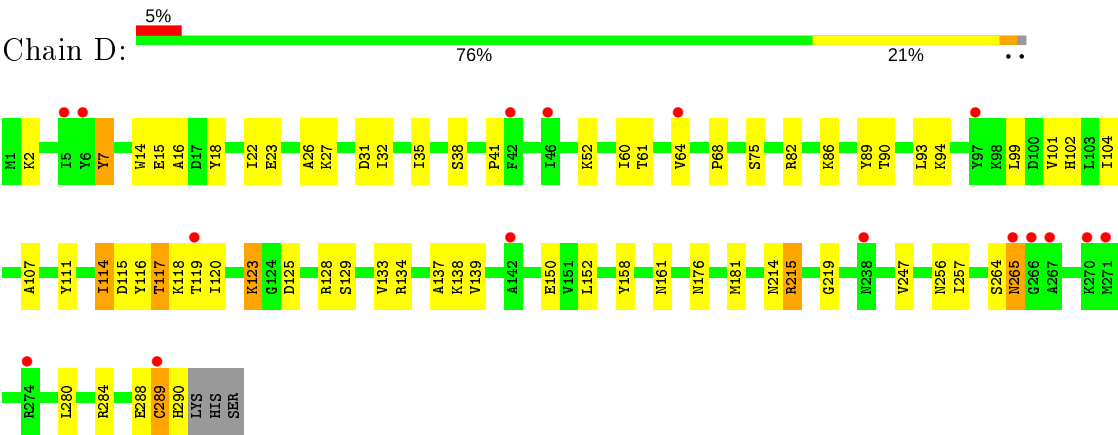
- Molecule 1: Xylose isomerase domain protein TIM barrel



- Molecule 1: Xylose isomerase domain protein TIM barrel



● Molecule 1: Xylose isomerase domain protein TIM barrel



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.92Å 115.22Å 91.61Å 90.00° 105.73° 90.00°	Depositor
Resolution (Å)	25.00 – 2.12 24.76 – 2.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.12) 94.0 (24.76-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.190 , 0.232 0.188 , 0.232	Depositor DCC
R_{free} test set	4327 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9870	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: SDD, MN

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	0.76	0/2344	0.84	3/3173 (0.1%)
1	B	0.68	0/2357	0.79	1/3192 (0.0%)
1	C	0.61	0/2340	0.79	1/3169 (0.0%)
1	D	0.64	0/2357	0.77	2/3192 (0.1%)
All	All	0.68	0/9398	0.80	7/12726 (0.1%)

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	B	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	220	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	215	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	215	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	273	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	268	ASP	CB-CG-OD1	5.18	122.97	118.30
1	D	219	GLY	N-CA-C	5.05	125.74	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	TYR	Sidechain
1	B	7	TYR	Sidechain
1	D	158	TYR	Sidechain
1	D	7	TYR	Sidechain

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	2292	0	2223	41	0
1	B	2303	0	2235	57	0
1	C	2287	0	2223	49	0
1	D	2303	0	2235	47	0
2	A	12	0	12	1	0
2	B	12	0	11	0	0
2	C	12	0	12	1	0
2	D	12	0	11	1	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	213	0	0	8	0
4	B	157	0	0	3	0
4	C	123	0	0	4	0
4	D	136	0	0	3	0
All	All	9870	0	8962	192	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 11.

All (192) 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:176:ASN:ND2	1:B:176:ASN:H	1.46	1.05
1:B:118:LYS:HE2	1:B:118:LYS:HA	1.40	1.03
1:D:115:ASP:OD2	1:D:117:THR:HB	1.63	0.99
1:D:90:THR:HG22	1:D:139:VAL:HG21	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ARG:NH2	1:D:288:GLU:O	2.04	0.90
1:B:176:ASN:N	1:B:176:ASN:HD22	1.71	0.88
1:B:175:HIS:HD2	1:B:177:ASN:H	1.24	0.84
1:B:47:GLN:HA	1:B:50:GLU:HG3	1.57	0.84
1:B:25:VAL:HG13	1:B:30:PHE:HB2	1.59	0.83
1:A:1:MET:CA	1:A:1:MET:CG	2.56	0.83
1:B:189:ILE:HG12	1:C:189:ILE:CD1	2.09	0.83
1:B:176:ASN:HD22	1:B:176:ASN:H	0.87	0.81
1:B:176:ASN:N	1:B:176:ASN:ND2	2.28	0.81
1:B:86:LYS:O	1:B:90:THR:HG23	1.82	0.80
1:B:189:ILE:HG12	1:C:189:ILE:HD11	1.66	0.78
1:B:96:LEU:HG	1:B:101:VAL:CG2	2.15	0.77
1:A:114:ILE:HD13	1:A:157:ASN:HA	1.67	0.76
1:C:25:VAL:HG13	1:C:30:PHE:HB2	1.69	0.75
1:A:125:ASP:HA	1:A:128:ARG:NH1	2.02	0.75
1:D:23:GLU:O	1:D:27:LYS:HG2	1.87	0.74
1:A:83:LYS:HE3	1:A:83:LYS:O	1.87	0.74
1:C:175:HIS:CD2	1:C:177:ASN:H	2.05	0.74
1:C:118:LYS:HE2	1:C:119:THR:H	1.54	0.72
1:B:74:LEU:HD23	1:B:85:ALA:HB1	1.72	0.71
1:D:102:HIS:NE2	4:D:459:HOH:O	2.23	0.70
1:B:96:LEU:HG	1:B:101:VAL:HG22	1.73	0.69
1:A:125:ASP:HA	1:A:128:ARG:HH12	1.57	0.69
1:C:102:HIS:NE2	4:C:523:HOH:O	2.26	0.69
1:C:14:TRP:HE1	1:C:256:ASN:ND2	1.91	0.68
1:C:175:HIS:HD2	1:C:177:ASN:H	1.41	0.68
1:D:289:CYS:O	1:D:290:HIS:HB2	1.93	0.68
1:B:217:VAL:HG12	1:B:245:PRO:HG3	1.76	0.67
1:D:38:SER:O	1:D:41:PRO:HD2	1.93	0.67
1:B:175:HIS:CD2	1:B:177:ASN:H	2.10	0.66
1:C:118:LYS:CE	1:C:119:THR:H	2.09	0.66
1:B:150:GLU:HA	1:B:181:MET:HB3	1.78	0.64
1:B:114:ILE:HD12	1:B:157:ASN:HA	1.79	0.64
1:B:274:ARG:HB3	1:B:274:ARG:NH1	2.11	0.64
1:C:112:TRP:CH2	1:C:256:ASN:HB3	2.33	0.63
1:D:82:ARG:O	1:D:86:LYS:HG3	1.99	0.63
1:B:189:ILE:HG12	1:C:189:ILE:HD12	1.79	0.63
1:A:14:TRP:HE1	1:A:256:ASN:ND2	1.98	0.62
1:D:111:TYR:CE2	1:D:114:ILE:HA	2.34	0.62
1:C:175:HIS:HD2	1:C:176:ASN:N	1.98	0.62
1:A:115:ASP:OD1	1:A:117:THR:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:ND2	1:A:238:ASN:H	1.99	0.60
1:B:96:LEU:HG	1:B:101:VAL:HG21	1.83	0.60
1:C:126:TRP:O	1:C:130:VAL:HG23	2.02	0.60
1:C:244:GLU:O	1:C:244:GLU:HG2	2.03	0.59
1:B:102:HIS:NE2	4:B:438:HOH:O	2.31	0.59
1:C:175:HIS:CD2	1:C:176:ASN:N	2.70	0.59
1:A:215:ARG:HD2	4:A:612:HOH:O	2.03	0.58
1:D:118:LYS:HE3	1:D:119:THR:H	1.66	0.58
1:A:123:LYS:HG2	4:A:606:HOH:O	2.02	0.58
1:A:123:LYS:HE2	4:A:522:HOH:O	2.03	0.58
1:C:14:TRP:CH2	1:C:253:VAL:HG22	2.39	0.57
1:D:14:TRP:HE1	1:D:256:ASN:ND2	2.02	0.57
1:A:103:LEU:HD23	1:A:103:LEU:C	2.25	0.57
1:A:66:HIS:HD2	4:A:613:HOH:O	1.87	0.56
1:C:18:TYR:O	1:C:22:ILE:HG13	2.06	0.56
1:D:2:LYS:N	1:D:2:LYS:HD2	2.21	0.56
1:B:270:LYS:NZ	1:B:274:ARG:HD2	2.21	0.56
1:C:114:ILE:HD12	1:C:157:ASN:HA	1.87	0.56
1:B:74:LEU:HD23	1:B:85:ALA:CB	2.36	0.55
1:C:14:TRP:HE1	1:C:256:ASN:HD22	1.53	0.55
1:D:31:ASP:OD2	1:D:284:ARG:NH2	2.39	0.55
1:A:75:SER:O	1:A:128:ARG:NH1	2.39	0.54
1:D:114:ILE:HD11	1:D:116:TYR:CE2	2.41	0.54
1:B:38:SER:O	1:B:41:PRO:HD2	2.06	0.54
1:D:289:CYS:O	1:D:290:HIS:CB	2.55	0.54
1:C:9:TYR:CD1	1:C:245:PRO:HG2	2.41	0.54
1:A:68:PRO:HB2	1:A:111:TYR:HA	1.89	0.54
1:D:90:THR:HA	1:D:139:VAL:HG11	1.89	0.54
1:D:86:LYS:O	1:D:90:THR:HG23	2.08	0.53
1:D:32:ILE:HG12	1:D:61:THR:HB	1.89	0.53
1:D:123:LYS:HE3	1:D:123:LYS:HA	1.91	0.53
1:C:1:MET:HB3	1:C:288:GLU:OE2	2.09	0.52
1:A:244:GLU:HG2	1:A:246:PHE:CE2	2.45	0.52
2:A:301:SDD:H4	2:A:301:SDD:O6	2.10	0.52
1:A:100:ASP:HA	4:A:609:HOH:O	2.10	0.52
1:A:14:TRP:HE1	1:A:256:ASN:HD22	1.57	0.52
1:D:18:TYR:O	1:D:22:ILE:HG13	2.10	0.52
1:D:257:ILE:HG22	1:D:257:ILE:O	2.10	0.52
1:D:289:CYS:HA	4:D:535:HOH:O	2.09	0.52
1:B:43:TYR:HB3	1:B:48:ILE:HG13	1.93	0.51
1:C:7:TYR:CG	1:C:8:ALA:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PRO:HA	1:B:128:ARG:HD3	1.92	0.50
1:C:150:GLU:HA	1:C:181:MET:HB3	1.93	0.50
1:D:68:PRO:HB2	1:D:111:TYR:HA	1.93	0.50
1:A:138:LYS:HD2	4:A:565:HOH:O	2.12	0.50
1:B:173:VAL:HG11	1:B:178:VAL:HG21	1.92	0.50
1:D:89:TYR:O	1:D:93:LEU:HD13	2.12	0.50
1:A:238:ASN:H	1:A:238:ASN:HD22	1.59	0.49
1:A:256:ASN:ND2	4:A:454:HOH:O	2.42	0.49
1:B:9:TYR:CD1	1:B:245:PRO:HG2	2.47	0.49
1:C:69:SER:OG	1:C:72:GLN:HG3	2.12	0.49
1:A:109:TYR:HE1	1:A:157:ASN:HD21	1.60	0.49
1:A:215:ARG:CD	4:A:612:HOH:O	2.60	0.49
1:C:74:LEU:HD22	1:C:132:SER:HB3	1.94	0.49
1:C:175:HIS:C	1:C:175:HIS:CD2	2.86	0.49
1:D:26:ALA:HA	1:D:60:ILE:HD11	1.94	0.48
1:B:189:ILE:CG1	1:C:189:ILE:HD12	2.42	0.48
1:B:274:ARG:HH11	1:B:274:ARG:CB	2.25	0.48
1:B:74:LEU:HB3	1:B:132:SER:HB3	1.95	0.47
1:C:135:GLU:O	1:C:138:LYS:HB2	2.13	0.47
1:B:126:TRP:O	1:B:130:VAL:HG23	2.14	0.47
1:B:134:ARG:O	1:B:137:ALA:HB3	2.14	0.47
1:B:274:ARG:HB3	1:B:274:ARG:HH11	1.79	0.47
1:D:15:GLU:O	1:D:16:ALA:HB2	2.14	0.47
1:B:44:SER:H	1:B:47:GLN:CG	2.28	0.47
1:B:32:ILE:CG2	1:B:33:LEU:N	2.77	0.47
1:D:64:VAL:O	1:D:104:ILE:HA	2.14	0.47
1:A:66:HIS:HE1	1:A:72:GLN:OE1	1.98	0.46
1:D:75:SER:O	1:D:128:ARG:HD2	2.15	0.46
1:B:205:LEU:HD13	1:B:237:TYR:CE1	2.51	0.46
1:D:14:TRP:HE1	1:D:256:ASN:HD22	1.63	0.46
1:B:176:ASN:HB3	4:B:500:HOH:O	2.15	0.46
1:D:115:ASP:C	1:D:117:THR:H	2.18	0.46
1:B:68:PRO:HB2	1:B:111:TYR:HA	1.98	0.45
1:C:4:GLY:HA3	1:C:32:ILE:HB	1.98	0.45
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.31	0.45
1:B:37:ALA:HB2	1:B:64:VAL:CG1	2.46	0.45
1:D:90:THR:O	1:D:94:LYS:HG2	2.17	0.45
1:C:107:ALA:HB2	1:C:152:LEU:HD11	1.98	0.44
1:D:125:ASP:OD1	1:D:128:ARG:NH1	2.50	0.44
1:C:95:ARG:NH2	4:C:431:HOH:O	2.50	0.44
1:B:107:ALA:HB2	1:B:152:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:VAL:CG1	1:C:171:LYS:HE2	2.47	0.44
1:D:150:GLU:HA	1:D:181:MET:HB3	2.00	0.44
1:A:120:ILE:HD12	1:A:158:TYR:CE2	2.52	0.44
1:C:2:LYS:HD3	1:C:2:LYS:HA	1.80	0.44
1:B:51:LEU:HB3	1:B:99:LEU:HD11	1.99	0.44
1:A:114:ILE:CD1	1:A:157:ASN:HA	2.45	0.44
1:C:100:ASP:OD1	4:C:523:HOH:O	2.21	0.44
1:A:7:TYR:CG	1:A:8:ALA:N	2.86	0.44
1:B:19:LYS:O	1:B:23:GLU:HG3	2.18	0.44
1:C:103:LEU:C	1:C:103:LEU:HD23	2.38	0.44
1:D:247:VAL:HG23	1:D:264:SER:HB3	2.00	0.44
1:A:214:ASN:O	1:A:215:ARG:HB2	2.18	0.44
1:B:75:SER:O	1:B:128:ARG:HD2	2.18	0.44
1:D:134:ARG:O	1:D:137:ALA:HB3	2.16	0.44
1:D:107:ALA:HB2	1:D:152:LEU:HD11	2.00	0.43
1:A:74:LEU:HD22	1:A:132:SER:HB3	2.00	0.43
1:A:270:LYS:HA	1:A:270:LYS:HD2	1.81	0.43
1:D:265:ASN:HD22	1:D:265:ASN:C	2.22	0.43
1:A:7:TYR:OH	1:A:14:TRP:HA	2.17	0.43
1:D:31:ASP:CG	1:D:284:ARG:NH2	2.72	0.43
1:C:247:VAL:HG23	1:C:264:SER:HB3	2.00	0.43
1:D:129:SER:O	1:D:133:VAL:HG23	2.19	0.43
1:A:30:PHE:CE1	1:A:280:LEU:HG	2.54	0.43
1:A:238:ASN:N	1:A:238:ASN:ND2	2.56	0.42
1:A:271:MET:CE	1:A:274:ARG:HH22	2.32	0.42
1:B:244:GLU:HG2	1:B:246:PHE:CE2	2.55	0.42
1:C:120:ILE:HD12	1:C:158:TYR:CE2	2.55	0.42
1:B:110:SER:OG	1:B:111:TYR:N	2.51	0.42
1:B:15:GLU:O	1:B:16:ALA:HB2	2.20	0.42
1:B:94:LYS:HD2	1:B:143:CYS:SG	2.60	0.42
1:C:280:LEU:HD21	1:C:284:ARG:HH12	1.83	0.42
1:A:271:MET:SD	1:A:274:ARG:NH2	2.93	0.42
1:B:289:CYS:HA	4:B:492:HOH:O	2.19	0.42
1:A:209:HIS:HA	1:A:242:VAL:O	2.20	0.42
1:B:14:TRP:CZ2	1:B:253:VAL:HG22	2.54	0.42
1:D:214:ASN:O	1:D:215:ARG:HB2	2.19	0.42
1:C:84:ASN:HD22	1:C:84:ASN:N	2.18	0.41
1:B:262:ASP:OD2	1:B:266:GLY:N	2.52	0.41
1:B:32:ILE:HG12	1:B:61:THR:HB	2.02	0.41
1:B:44:SER:OG	1:B:47:GLN:HG2	2.19	0.41
1:D:52:LYS:HB2	1:D:99:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HG2	1:A:220:ARG:HH11	1.86	0.41
1:B:37:ALA:HB2	1:B:64:VAL:HG11	2.03	0.41
2:D:301:SDD:H11	2:D:301:SDD:H4	1.88	0.41
1:C:261:ARG:HG3	1:C:263:ILE:HG13	2.02	0.41
1:C:84:ASN:ND2	1:C:84:ASN:N	2.68	0.41
1:A:27:LYS:HA	1:A:27:LYS:HD3	1.87	0.41
1:B:290:HIS:HA	4:D:509:HOH:O	2.20	0.41
1:A:181:MET:CE	1:A:209:HIS:CE1	3.04	0.41
1:C:253:VAL:O	1:C:257:ILE:HG12	2.21	0.41
2:C:301:SDD:H4	2:C:301:SDD:O6	2.20	0.41
1:C:96:LEU:HG	1:C:101:VAL:CG1	2.51	0.41
1:A:99:LEU:HB3	1:A:101:VAL:HG23	2.03	0.40
1:C:14:TRP:CZ2	1:C:253:VAL:HG22	2.56	0.40
1:C:284:ARG:O	1:C:288:GLU:HG3	2.21	0.40
1:D:99:LEU:HB3	1:D:101:VAL:HG23	2.03	0.40
1:C:215:ARG:HD2	4:C:520:HOH:O	2.20	0.40
1:D:284:ARG:O	1:D:288:GLU:HB2	2.21	0.40
1:C:10:TRP:CZ2	1:C:24:LYS:HD3	2.56	0.40
1:D:152:LEU:O	1:D:161:ASN:HA	2.21	0.40
1:D:117:THR:HG22	1:D:118:LYS:N	2.37	0.40
1:D:7:TYR:HD1	1:D:35:ILE:HA	1.84	0.40
1:B:18:TYR:CZ	1:B:35:ILE:HB	2.56	0.40
1:C:40:LEU:N	1:C:41:PRO:CD	2.84	0.40
1:D:23:GLU:O	1:D:27:LYS:CG	2.66	0.40

There are no symmetry-related clashes.

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	287/293 (98%)	275 (96%)	12 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	288/293 (98%)	275 (96%)	13 (4%)	0	100	100
1	C	286/293 (98%)	276 (96%)	9 (3%)	1 (0%)	41	40
1	D	288/293 (98%)	271 (94%)	16 (6%)	1 (0%)	41	40
All	All	1149/1172 (98%)	1097 (96%)	50 (4%)	2 (0%)	47	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	239	GLY
1	D	289	CYS

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	240/245 (98%)	227 (95%)	13 (5%)	22	19
1	B	242/245 (99%)	234 (97%)	8 (3%)	38	39
1	C	240/245 (98%)	235 (98%)	5 (2%)	53	57
1	D	242/245 (99%)	234 (97%)	8 (3%)	38	39
All	All	964/980 (98%)	930 (96%)	34 (4%)	36	37

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	62	LEU
1	A	83	LYS
1	A	96	LEU
1	A	99	LEU
1	A	114	ILE
1	A	118	LYS
1	A	134	ARG
1	A	141	GLU

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Mol	Chain	Res	Type
1	A	175	HIS
1	A	238	ASN
1	A	272	LEU
1	A	280	LEU
1	B	47	GLN
1	B	50	GLU
1	B	96	LEU
1	B	101	VAL
1	B	114	ILE
1	B	176	ASN
1	B	205	LEU
1	B	265	ASN
1	C	71	GLU
1	C	99	LEU
1	C	114	ILE
1	C	118	LYS
1	C	159	LEU
1	D	114	ILE
1	D	117	THR
1	D	120	ILE
1	D	123	LYS
1	D	138	LYS
1	D	176	ASN
1	D	265	ASN
1	D	280	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	66	HIS
1	A	157	ASN
1	A	238	ASN
1	A	256	ASN
1	A	277	GLN
1	B	12	GLN
1	B	161	ASN
1	B	175	HIS
1	B	176	ASN
1	B	256	ASN
1	C	66	HIS
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	175	HIS
1	C	177	ASN
1	C	256	ASN
1	D	12	GLN
1	D	84	ASN
1	D	177	ASN
1	D	256	ASN
1	D	265	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	SDD	C	301	3	10,11,11	0.57	0	9,14,14	0.58	0
2	SDD	B	301	3	10,11,11	0.58	0	9,14,14	0.82	0
2	SDD	D	301	3	10,11,11	0.58	0	9,14,14	1.28	1 (11%)
2	SDD	A	301	3	10,11,11	0.58	0	9,14,14	0.78	0

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	SDD	C	301	3	-	6/16/16/16	-
2	SDD	B	301	3	-	2/16/16/16	-
2	SDD	D	301	3	-	0/16/16/16	-
2	SDD	A	301	3	-	2/16/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	301	SDD	C6-C5-C4	-2.28	107.46	112.41

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SDD	O1-C1-C2-O2
2	C	301	SDD	O1-C1-C2-O2
2	C	301	SDD	C1-C2-C3-C4
2	C	301	SDD	C3-C4-C5-O5
2	B	301	SDD	O5-C5-C6-O6
2	A	301	SDD	C1-C2-C3-C4
2	B	301	SDD	C1-C2-C3-C4
2	C	301	SDD	C3-C4-C5-C6
2	C	301	SDD	O4-C4-C5-O5
2	C	301	SDD	O4-C4-C5-C6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	SDD	1	0
2	D	301	SDD	1	0
2	A	301	SDD	1	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	289/293 (98%)	-0.08	8 (2%) 53 59	27, 39, 56, 78	0
1	B	290/293 (98%)	0.18	14 (4%) 30 35	29, 48, 67, 84	0
1	C	288/293 (98%)	0.18	11 (3%) 40 46	34, 49, 64, 83	0
1	D	290/293 (98%)	0.15	16 (5%) 25 30	32, 48, 67, 81	0
All	All	1157/1172 (98%)	0.11	49 (4%) 36 42	27, 46, 65, 84	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	ASN	5.2
1	B	117	THR	4.6
1	C	119	THR	4.1
1	B	119	THR	4.1
1	D	289	CYS	4.0
1	A	289	CYS	3.8
1	D	270	LYS	3.8
1	B	289	CYS	3.8
1	D	119	THR	3.7
1	A	118	LYS	3.7
1	A	117	THR	3.6
1	C	238	ASN	3.5
1	B	80	ASP	3.5
1	C	270	LYS	3.3
1	D	42	PHE	3.3
1	D	46	ILE	3.3
1	C	117	THR	3.1
1	B	238	ASN	3.1
1	C	176	ASN	2.9
1	C	252	THR	2.9
1	D	6	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	97	TYR	2.8
1	B	139	VAL	2.8
1	A	149	LEU	2.8
1	C	142	ALA	2.7
1	D	265	ASN	2.7
1	B	5	ILE	2.6
1	B	97	TYR	2.5
1	A	119	THR	2.5
1	B	265	ASN	2.5
1	D	271	MET	2.5
1	C	97	TYR	2.5
1	D	266	GLY	2.4
1	B	46	ILE	2.4
1	C	149	LEU	2.4
1	B	118	LYS	2.4
1	D	274	ARG	2.4
1	C	106	GLY	2.4
1	B	270	LYS	2.3
1	D	64	VAL	2.3
1	B	110	SER	2.3
1	D	267	ALA	2.2
1	A	271	MET	2.2
1	C	27	LYS	2.2
1	B	274	ARG	2.2
1	A	265	ASN	2.1
1	D	5	ILE	2.1
1	A	235	ILE	2.0
1	D	142	ALA	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(Å ²)	Q<0.9
2	SDD	D	301	12/12	0.85	0.19	42,47,51,54	0
3	MN	C	303	1/1	0.87	0.17	72,72,72,72	0
2	SDD	C	301	12/12	0.92	0.14	47,52,54,59	0
2	SDD	A	301	12/12	0.93	0.16	38,44,46,49	0
2	SDD	B	301	12/12	0.95	0.12	43,46,47,53	0
3	MN	A	303	1/1	0.98	0.10	71,71,71,71	0
3	MN	B	304	1/1	0.98	0.03	49,49,49,49	0
3	MN	B	303	1/1	0.99	0.02	50,50,50,50	0
3	MN	D	302	1/1	0.99	0.12	36,36,36,36	0
3	MN	A	302	1/1	0.99	0.09	33,33,33,33	0
3	MN	B	302	1/1	1.00	0.09	35,35,35,35	0
3	MN	C	302	1/1	1.00	0.12	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.