



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 05:53 PM EDT

PDB ID : 3VNI
Title : Crystal structures of D-Psicose 3-epimerase from *Clostridium cellulolyticum* H10 and its complex with ketohexose sugars
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 : 2012-01-16
Resolution : 1.98 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 : 4.02b-467
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

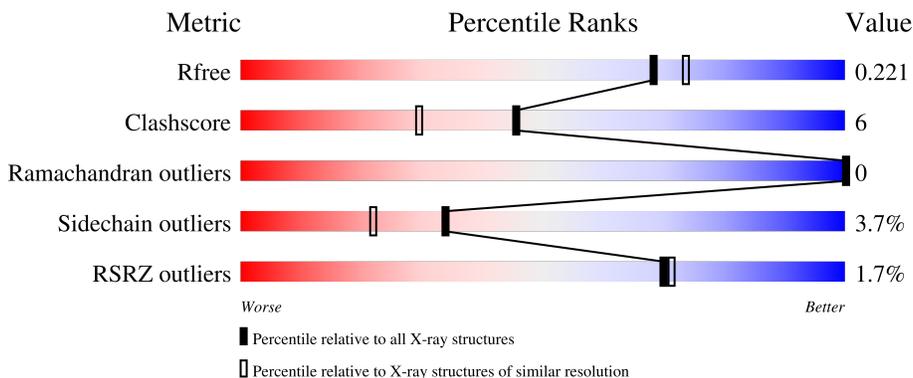
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	294	 2% 82% 15% ..
1	B	294	 2% 83% 12% ..
1	C	294	 % 86% 11% ..
1	D	294	 2% 83% 14% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10344 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
			Total	C	N	O	S			
1	A	289	2293	1459	388	435	11	0	0	0
1	B	289	2292	1459	388	435	10	0	0	0
1	C	288	2287	1456	387	434	10	0	0	0
1	D	288	2287	1456	387	434	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

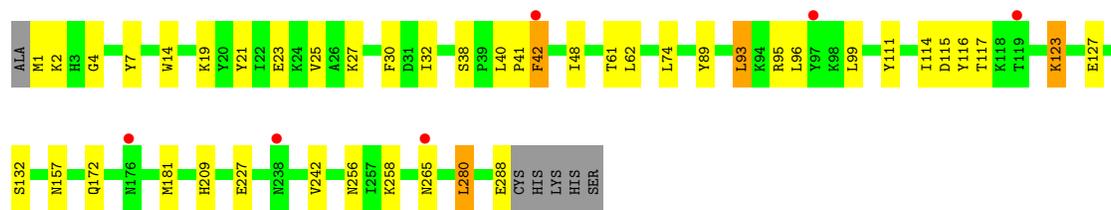
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP B8I944
B	0	ALA	-	expression tag	UNP B8I944
C	0	ALA	-	expression tag	UNP B8I944
D	0	ALA	-	expression tag	UNP B8I944

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	339	Total 339	O 339	0	0
3	B	282	Total 282	O 282	0	0
3	C	295	Total 295	O 295	0	0
3	D	265	Total 265	O 265	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.76Å 115.44Å 91.63Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	25.00 – 1.98 24.74 – 1.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-1.98) 93.5 (24.74-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.98Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.175 , 0.220 0.176 , 0.221	Depositor DCC
R_{free} test set	5270 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10344	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.88	1/2346 (0.0%)	0.84	2/3177 (0.1%)
1	B	0.76	0/2345	0.78	1/3176 (0.0%)
1	C	0.75	1/2340 (0.0%)	0.79	1/3169 (0.0%)
1	D	0.73	0/2340	0.79	0/3169
All	All	0.78	2/9371 (0.0%)	0.80	4/12691 (0.0%)

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	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLU	CD-OE1	6.80	1.33	1.25
1	C	34	GLU	CD-OE1	6.12	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	176	ASN	N-CA-C	5.37	125.50	111.00
1	A	128	ARG	NE-CZ-NH1	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ASN	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	TYR	Sidechain
1	B	7	TYR	Sidechain
1	C	21	TYR	Sidechain
1	C	7	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	2293	0	2228	30	0
1	B	2292	0	2228	40	0
1	C	2287	0	2223	24	0
1	D	2287	0	2223	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	339	0	0	6	1
3	B	282	0	0	1	0
3	C	295	0	0	0	0
3	D	265	0	0	3	1
All	All	10344	0	8902	116	1

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 6.

All (116) 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:C:118:LYS:HA	1:C:118:LYS:HE2	1.57	0.86
1:A:75:SER:O	1:A:128:ARG:NH1	2.13	0.81
1:D:123:LYS:HE3	1:D:123:LYS:HA	1.62	0.81
1:D:14:TRP:HE1	1:D:256:ASN:HD22	1.29	0.81
1:D:23:GLU:O	1:D:27:LYS:HG2	1.81	0.80
1:A:98:LYS:HD3	3:A:7402:HOH:O	1.84	0.77
1:D:32:ILE:HD13	1:D:61:THR:HB	1.66	0.77
1:C:157:ASN:HD22	1:C:158:TYR:H	1.33	0.77
1:A:14:TRP:HE1	1:A:256:ASN:HD22	1.35	0.74
1:D:4:GLY:HA3	1:D:32:ILE:HB	1.71	0.72
1:C:25:VAL:HG13	1:C:30:PHE:HB2	1.71	0.72
1:B:274:ARG:CG	1:B:274:ARG:HH11	2.03	0.71
1:B:14:TRP:HE1	1:B:256:ASN:HD22	1.39	0.69
1:B:270:LYS:NZ	1:B:274:ARG:HE	1.92	0.67
1:A:271:MET:HE2	1:A:275:GLU:HG2	1.76	0.67
1:B:274:ARG:HH11	1:B:274:ARG:CB	2.08	0.67
1:A:1:MET:HE2	1:A:288:GLU:HG2	1.78	0.66
1:D:123:LYS:O	1:D:127:GLU:HG2	1.94	0.66
1:C:14:TRP:HE1	1:C:256:ASN:HD22	1.44	0.66
1:A:14:TRP:HE1	1:A:256:ASN:ND2	1.95	0.65
1:B:274:ARG:NH1	1:B:274:ARG:HG2	2.11	0.64
1:C:157:ASN:ND2	1:C:158:TYR:H	1.96	0.64
1:A:115:ASP:OD2	1:A:117:THR:HB	1.98	0.64
1:A:289:CYS:HB3	3:A:7321:HOH:O	1.98	0.63
1:D:14:TRP:HE1	1:D:256:ASN:ND2	1.94	0.63
1:B:14:TRP:HE1	1:B:256:ASN:ND2	1.97	0.62
1:A:66:HIS:HD2	3:A:7421:HOH:O	1.81	0.61
1:C:284:ARG:O	1:C:288:GLU:HG3	2.01	0.60
1:C:14:TRP:HE1	1:C:256:ASN:ND2	1.98	0.60
1:B:274:ARG:HH11	1:B:274:ARG:HG2	1.66	0.59
1:B:270:LYS:HZ3	1:B:274:ARG:HE	1.50	0.59
1:C:150:GLU:HB2	1:C:181:MET:HE2	1.85	0.57
1:C:157:ASN:HD22	1:C:158:TYR:N	2.02	0.57
1:A:271:MET:HE2	1:A:275:GLU:CG	2.35	0.57
1:C:150:GLU:HB2	1:C:181:MET:CE	2.35	0.57
1:D:115:ASP:OD2	1:D:117:THR:HB	2.05	0.56
1:B:25:VAL:HG13	1:B:30:PHE:HB2	1.86	0.56
1:A:150:GLU:HB2	1:A:181:MET:CE	2.36	0.55
1:D:1:MET:HG3	1:D:288:GLU:OE2	2.05	0.55
1:A:1:MET:N	3:A:7183:HOH:O	2.40	0.55
1:A:46:ILE:O	1:A:50:GLU:HG3	2.06	0.55
1:D:181:MET:CE	1:D:209:HIS:CE1	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HG2	1:A:246:PHE:CE2	2.43	0.54
1:B:107:ALA:HB2	1:B:152:LEU:HD11	1.89	0.53
3:A:7431:HOH:O	1:D:258:LYS:HE2	2.07	0.53
1:D:42:PHE:CD1	1:D:42:PHE:N	2.72	0.53
1:B:47:GLN:HA	1:B:50:GLU:HG2	1.91	0.53
1:D:48:ILE:HD11	1:D:95:ARG:HH11	1.74	0.52
1:C:115:ASP:OD2	1:C:118:LYS:HG2	2.10	0.52
1:D:227:GLU:OE1	3:D:644:HOH:O	2.19	0.51
1:D:181:MET:HE3	1:D:209:HIS:CE1	2.45	0.51
1:D:172:GLN:HG3	3:D:549:HOH:O	2.12	0.50
1:B:9:TYR:CD1	1:B:245:PRO:HG2	2.48	0.48
1:B:94:LYS:HD2	1:B:143:CYS:SG	2.53	0.48
1:D:209:HIS:HA	1:D:242:VAL:O	2.14	0.48
1:B:150:GLU:HB2	1:B:181:MET:HE1	1.96	0.47
1:A:5:ILE:HG13	1:A:243:MET:HG3	1.96	0.47
1:C:37:ALA:HB2	1:C:64:VAL:CG1	2.44	0.47
1:C:107:ALA:HB2	1:C:152:LEU:HD11	1.97	0.47
1:B:44:SER:H	1:B:47:GLN:CG	2.27	0.47
1:A:150:GLU:HB2	1:A:181:MET:HE2	1.97	0.47
1:C:237:TYR:CZ	1:C:239:GLY:HA3	2.50	0.47
1:D:38:SER:O	1:D:41:PRO:HD2	2.15	0.47
1:D:89:TYR:O	1:D:93:LEU:HB2	2.15	0.47
1:D:74:LEU:HD22	1:D:132:SER:HB3	1.96	0.46
1:B:177:ASN:HD22	1:B:177:ASN:N	2.14	0.46
1:D:40:LEU:HB2	1:D:41:PRO:HD3	1.97	0.46
1:C:157:ASN:ND2	1:C:158:TYR:N	2.62	0.46
1:B:21:TYR:O	1:B:25:VAL:HB	2.16	0.46
1:B:260:TRP:CD1	1:C:158:TYR:HA	2.51	0.45
1:A:124:GLY:O	1:A:127:GLU:HG2	2.16	0.45
1:B:270:LYS:NZ	1:B:274:ARG:NE	2.64	0.45
1:B:288:GLU:O	3:B:479:HOH:O	2.21	0.45
1:B:42:PHE:CD1	1:B:42:PHE:N	2.84	0.45
1:A:271:MET:CE	1:A:275:GLU:HG2	2.45	0.45
1:B:150:GLU:HB2	1:B:181:MET:CE	2.46	0.45
1:A:271:MET:CE	1:A:274:ARG:NH1	2.80	0.45
1:B:116:TYR:CE1	1:C:260:TRP:CZ2	3.05	0.45
1:B:96:LEU:HG	1:B:101:VAL:HG22	1.98	0.45
1:C:118:LYS:HE2	1:C:118:LYS:CA	2.34	0.45
1:B:4:GLY:HA3	1:B:32:ILE:HB	1.99	0.44
1:B:157:ASN:ND2	1:B:158:TYR:H	2.15	0.44
1:C:120:ILE:HD12	1:C:158:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:OE1	1:A:152:LEU:HD21	2.18	0.44
1:A:30:PHE:CE1	1:A:280:LEU:HG	2.53	0.44
1:A:150:GLU:HB2	1:A:181:MET:HE3	1.99	0.44
1:B:274:ARG:HH11	1:B:274:ARG:HB2	1.83	0.44
1:D:21:TYR:O	1:D:25:VAL:HG22	2.18	0.44
1:A:238:ASN:C	3:A:7420:HOH:O	2.55	0.43
1:B:43:TYR:HA	1:B:47:GLN:OE1	2.18	0.43
1:A:86:LYS:NZ	1:A:135:GLU:OE2	2.38	0.43
1:B:212:GLU:CD	1:B:221:GLY:HA3	2.38	0.43
1:A:74:LEU:HD22	1:A:132:SER:HB3	2.00	0.43
1:B:44:SER:H	1:B:47:GLN:CD	2.22	0.43
1:C:177:ASN:N	1:C:177:ASN:HD22	2.17	0.43
1:B:244:GLU:HG2	1:B:246:PHE:CE2	2.54	0.43
1:B:176:ASN:HB3	1:B:177:ASN:HD22	1.83	0.42
1:B:26:ALA:HA	1:B:60:ILE:HD11	2.01	0.42
1:D:111:TYR:CE2	1:D:114:ILE:HA	2.54	0.42
1:B:118:LYS:HZ2	1:B:119:THR:H	1.65	0.42
1:B:114:ILE:O	1:B:114:ILE:HG13	2.19	0.42
1:B:270:LYS:HZ2	1:B:274:ARG:NE	2.18	0.42
1:B:173:VAL:HG11	1:B:178:VAL:HG21	2.02	0.42
1:A:271:MET:HE1	1:A:274:ARG:NH1	2.35	0.42
1:B:96:LEU:HG	1:B:101:VAL:CG2	2.50	0.41
1:C:99:LEU:O	1:C:100:ASP:HB3	2.20	0.41
1:D:30:PHE:CE1	1:D:280:LEU:HG	2.55	0.41
1:B:258:LYS:HG3	1:B:260:TRP:CZ2	2.56	0.41
1:C:7:TYR:CG	1:C:8:ALA:N	2.89	0.41
1:A:111:TYR:CE1	1:A:114:ILE:HG12	2.56	0.41
1:D:157:ASN:HB3	3:D:639:HOH:O	2.21	0.41
1:A:120:ILE:HD12	1:A:158:TYR:CE2	2.55	0.41
1:A:193:SER:HB2	1:C:230:GLU:OE2	2.20	0.41
1:C:78:ASP:OD1	1:C:78:ASP:C	2.60	0.41
1:B:42:PHE:H	1:B:42:PHE:HD1	1.67	0.40
1:A:103:LEU:HD23	1:A:103:LEU:C	2.42	0.40

All (1) 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)
3:A:7236:HOH:O	3:D:645:HOH:O[2_545]	2.19	0.01

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	287/294 (98%)	281 (98%)	6 (2%)	0	100	100
1	B	287/294 (98%)	278 (97%)	9 (3%)	0	100	100
1	C	286/294 (97%)	280 (98%)	6 (2%)	0	100	100
1	D	286/294 (97%)	279 (98%)	7 (2%)	0	100	100
All	All	1146/1176 (97%)	1118 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	241/245 (98%)	232 (96%)	9 (4%)	34	22
1	B	240/245 (98%)	231 (96%)	9 (4%)	33	21
1	C	240/245 (98%)	233 (97%)	7 (3%)	42	31
1	D	240/245 (98%)	229 (95%)	11 (5%)	27	14
All	All	961/980 (98%)	925 (96%)	36 (4%)	34	22

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	96	LEU
1	A	116	TYR
1	A	119	THR
1	A	270	LYS
1	A	272	LEU
1	A	280	LEU
1	A	289	CYS
1	B	25	VAL
1	B	42	PHE
1	B	47	GLN
1	B	96	LEU
1	B	116	TYR
1	B	118	LYS
1	B	205	LEU
1	B	258	LYS
1	B	274	ARG
1	C	1	MET
1	C	62	LEU
1	C	99	LEU
1	C	116	TYR
1	C	157	ASN
1	C	270	LYS
1	C	272	LEU
1	D	2	LYS
1	D	19	LYS
1	D	42	PHE
1	D	62	LEU
1	D	93	LEU
1	D	96	LEU
1	D	99	LEU
1	D	116	TYR
1	D	123	LYS
1	D	265	ASN
1	D	280	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	66	HIS
1	A	256	ASN
1	A	277	GLN

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Mol	Chain	Res	Type
1	B	12	GLN
1	B	176	ASN
1	B	177	ASN
1	B	256	ASN
1	C	49	ASN
1	C	66	HIS
1	C	84	ASN
1	C	157	ASN
1	C	177	ASN
1	C	256	ASN
1	D	12	GLN
1	D	177	ASN
1	D	256	ASN
1	D	265	ASN
1	D	277	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	289/294 (98%)	-0.40	5 (1%) 70 71	16, 23, 38, 58	0
1	B	289/294 (98%)	-0.20	5 (1%) 70 71	17, 27, 44, 58	0
1	C	288/294 (97%)	-0.24	4 (1%) 75 77	17, 28, 42, 62	0
1	D	288/294 (97%)	-0.11	6 (2%) 63 65	17, 30, 47, 61	0
All	All	1154/1176 (98%)	-0.24	20 (1%) 70 71	16, 27, 44, 62	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	PHE	7.3
1	B	0	ALA	4.8
1	C	119	THR	4.1
1	D	119	THR	3.7
1	A	289	CYS	3.4
1	D	265	ASN	3.3
1	B	42	PHE	3.2
1	C	238	ASN	2.9
1	D	238	ASN	2.8
1	A	117	THR	2.8
1	A	119	THR	2.7
1	B	265	ASN	2.7
1	C	117	THR	2.4
1	B	119	THR	2.4
1	B	142	ALA	2.3
1	C	118	LYS	2.2
1	A	265	ASN	2.1
1	A	118	LYS	2.1
1	D	97	TYR	2.0
1	D	176	ASN	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(\AA^2)	Q<0.9
2	MN	C	301	1/1	0.96	0.04	44,44,44,44	0
2	MN	A	7001	1/1	0.98	0.05	41,41,41,41	0
2	MN	B	301	1/1	0.99	0.03	37,37,37,37	0
2	MN	D	301	1/1	0.99	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.