



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 09:24 AM EST

PDB ID : 1ITW  
Title : Crystal structure of the monomeric isocitrate dehydrogenase in complex with isocitrate and Mn  
Authors : Yasutake, Y.; Watanabe, S.; Yao, M.; Takada, Y.; Fukunaga, N.; Tanaka, I.  
Deposited on : 2002-02-12  
Resolution : 1.95 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](mailto: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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

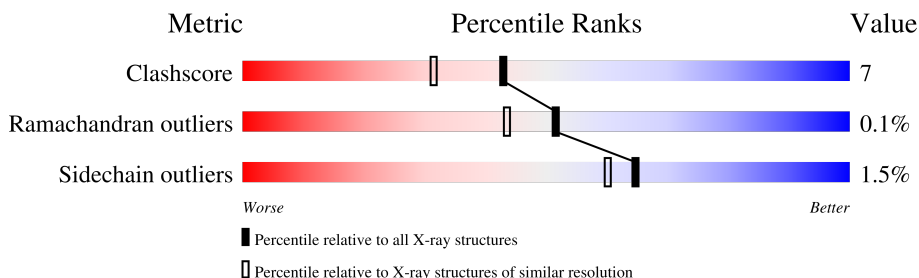
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	741	
1	B	741	
1	C	741	
1	D	741	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24949 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 Isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	740	5648	3568	969	1091	20	0	0	0
1	B	740	5648	3568	969	1091	20	0	0	0
1	C	739	5642	3565	968	1089	20	0	0	0
1	D	740	5648	3568	969	1091	20	0	0	0

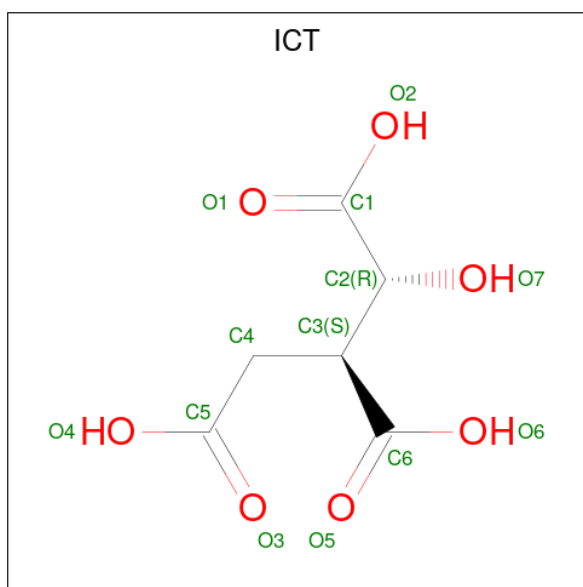
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	MET	ILE	SEE REMARK 999	UNP P16100
B	727	MET	ILE	SEE REMARK 999	UNP P16100
C	727	MET	ILE	SEE REMARK 999	UNP P16100
D	727	MET	ILE	SEE REMARK 999	UNP P16100

- 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	2	Total 2	Mn 2	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

- Molecule 3 is ISOCITRIC ACID (three-letter code: ICT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	724	Total O 724 724	0	0
4	B	606	Total O 606 606	0	0
4	C	322	Total O 322 322	0	0
4	D	654	Total O 654 654	0	0

### 3 Residue-property plots [i](#)

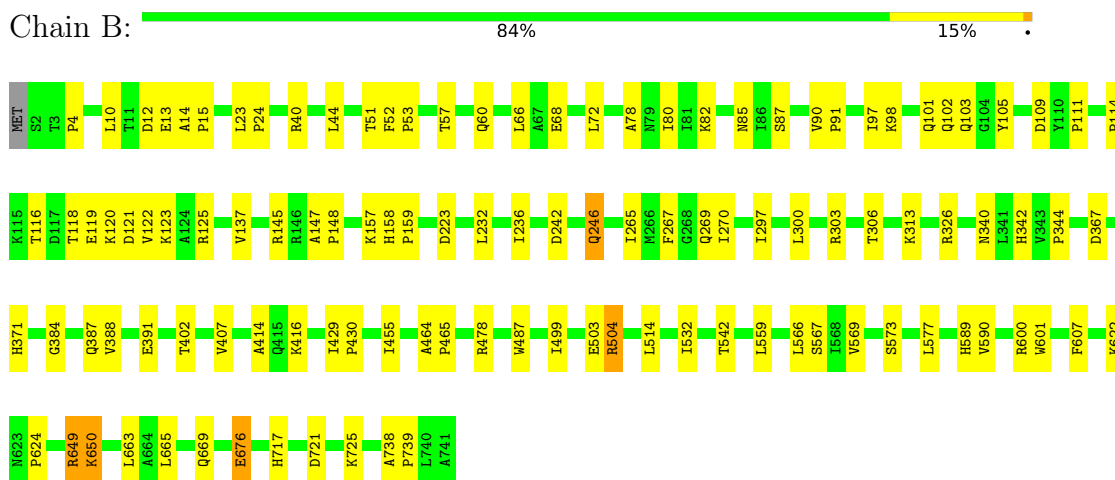
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

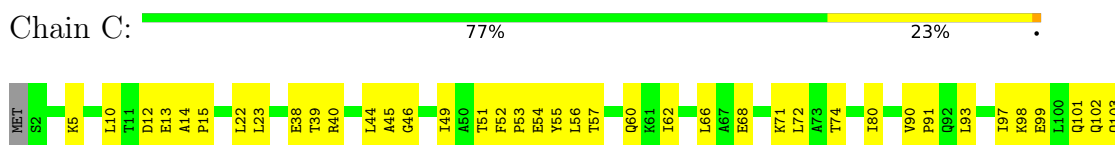
- Molecule 1: Isocitrate dehydrogenase

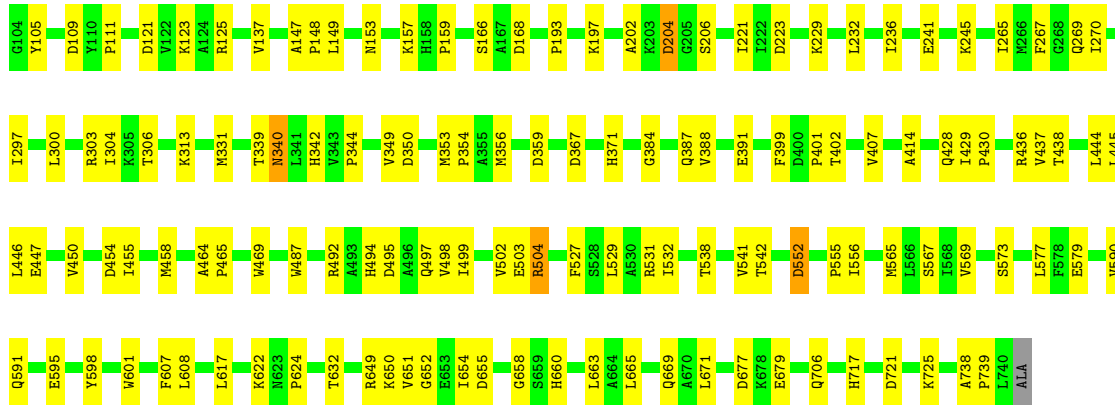


- Molecule 1: Isocitrate dehydrogenase



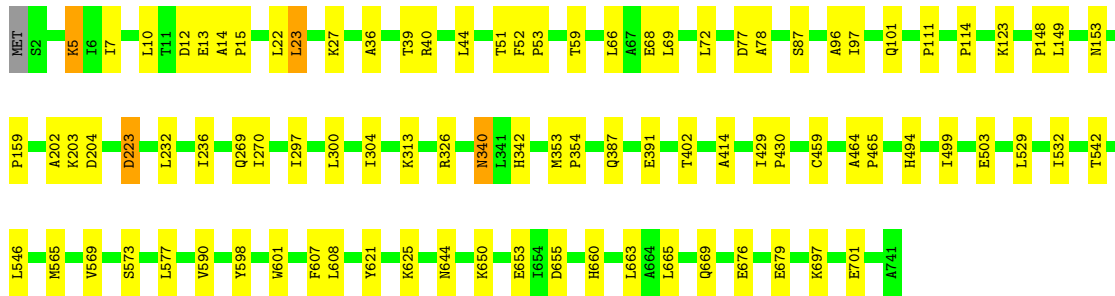
- Molecule 1: Isocitrate dehydrogenase





- Molecule 1: Isocitrate dehydrogenase

Chain D: 88% 12%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.41Å 119.02Å 128.22Å 90.00° 99.01° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95	Depositor
% Data completeness (in resolution range)	98.9 (10.00-1.95)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.193 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	24949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 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, ICT

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	0.31	0/5754	0.60	1/7798 (0.0%)
1	B	0.29	0/5754	0.57	1/7798 (0.0%)
1	C	0.26	0/5748	0.54	0/7791
1	D	0.30	0/5754	0.58	1/7798 (0.0%)
All	All	0.29	0/23010	0.57	3/31185 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	SER	N-CA-C	-5.81	95.32	111.00
1	B	87	SER	N-CA-C	-5.68	95.67	111.00
1	D	87	SER	N-CA-C	-5.65	95.75	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5648	0	5697	56	0
1	B	5648	0	5697	80	0
1	C	5642	0	5692	113	0
1	D	5648	0	5697	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	4	0	0
3	B	13	0	4	0	0
3	C	13	0	4	0	0
3	D	13	0	4	0	0
4	A	724	0	0	5	0
4	B	606	0	0	6	0
4	C	322	0	0	4	0
4	D	654	0	0	3	0
All	All	24949	0	22799	310	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 7.

All (310) 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:71:LYS:O	1:C:74:THR:HG22	1.68	0.93
1:C:202:ALA:HB3	1:C:206:SER:HB3	1.55	0.89
1:C:721:ASP:O	1:C:725:LYS:HD3	1.77	0.85
1:A:197:LYS:HE2	1:A:199:GLU:HG3	1.59	0.83
1:B:72:LEU:HD22	1:B:80:ILE:HD11	1.62	0.82
1:A:32:SER:HB3	1:A:683:GLN:HE22	1.46	0.80
1:B:721:ASP:O	1:B:725:LYS:HD3	1.85	0.76
1:C:464:ALA:HB3	1:C:465:PRO:HD3	1.69	0.74
1:C:654:ILE:HG23	1:C:658:GLY:HA3	1.71	0.73
1:C:72:LEU:HD22	1:C:80:ILE:HD11	1.70	0.73
1:A:741:ALA:HB2	4:A:1023:HOH:O	1.89	0.72
1:B:66:LEU:HD11	1:B:137:VAL:HG21	1.73	0.71
1:C:607:PHE:CE1	1:C:663:LEU:HD22	2.26	0.70
1:C:651:VAL:HG13	1:C:706:GLN:HB3	1.72	0.70
1:C:111:PRO:HG2	1:C:123:LYS:HB2	1.74	0.70
1:C:414:ALA:HB3	1:C:465:PRO:HB3	1.74	0.70
1:D:650:LYS:HB3	1:D:653:GLU:OE1	1.91	0.70
1:A:159:PRO:HG3	1:A:402:THR:HG22	1.72	0.70
1:A:152:LYS:HE3	1:A:156:ARG:NH1	2.08	0.69
1:C:591:GLN:O	1:C:595:GLU:HG3	1.92	0.69
1:C:555:PRO:HB3	1:C:565:MET:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:HD11	1:C:137:VAL:HG21	1.75	0.68
1:B:246:GLN:HE21	1:B:246:GLN:N	1.92	0.67
1:B:15:PRO:HG3	1:B:601:TRP:CZ2	2.30	0.66
1:C:438:THR:HG22	1:C:444:LEU:HA	1.77	0.66
1:B:121:ASP:O	1:B:125:ARG:HG2	1.95	0.66
1:B:504:ARG:C	1:B:504:ARG:HD3	2.16	0.66
1:B:478:ARG:HD3	1:B:514:LEU:HD11	1.77	0.65
1:B:159:PRO:HG3	1:B:402:THR:HG22	1.79	0.65
1:A:649:ARG:O	1:A:649:ARG:HG3	1.96	0.65
1:D:12:ASP:O	1:D:15:PRO:HD2	1.99	0.63
1:B:66:LEU:HD12	4:B:1315:HOH:O	1.99	0.62
1:C:445:LEU:C	1:C:446:LEU:HD12	2.18	0.62
1:C:241:GLU:HG2	4:C:757:HOH:O	1.98	0.62
1:C:297:ILE:HG22	1:C:342:HIS:HA	1.81	0.62
1:C:15:PRO:HG3	1:C:601:TRP:CH2	2.34	0.62
1:C:15:PRO:HG3	1:C:601:TRP:CZ2	2.35	0.62
1:B:103:GLN:OE1	1:B:717:HIS:HD2	1.82	0.62
1:B:236:ILE:HD13	1:B:270:ILE:HA	1.80	0.62
1:A:650:LYS:N	1:A:650:LYS:HD2	2.14	0.62
1:A:313:LYS:HB2	1:A:313:LYS:NZ	2.15	0.61
1:A:464:ALA:HB3	1:A:465:PRO:HD3	1.84	0.60
1:B:504:ARG:HD3	1:B:504:ARG:O	2.01	0.60
1:B:246:GLN:N	1:B:246:GLN:NE2	2.49	0.60
1:D:232:LEU:O	1:D:236:ILE:HG13	2.01	0.60
1:B:97:ILE:O	1:B:101:GLN:HG3	2.01	0.60
1:C:13:GLU:HB3	1:C:590:VAL:HG21	1.83	0.60
1:A:148:PRO:HD3	1:A:565:MET:HA	1.84	0.59
1:B:246:GLN:HE21	1:B:246:GLN:H	1.50	0.59
1:B:464:ALA:HB3	1:B:465:PRO:HD3	1.83	0.59
1:A:197:LYS:HE2	1:A:199:GLU:CG	2.30	0.59
1:B:303:ARG:O	1:B:306:THR:HG22	2.02	0.59
1:D:159:PRO:CG	1:D:402:THR:HG22	2.33	0.59
1:C:5:LYS:HD3	1:C:38:GLU:OE1	2.02	0.59
1:B:267:PHE:CD2	1:B:344:PRO:HG3	2.37	0.59
1:D:464:ALA:HB3	1:D:465:PRO:HD3	1.83	0.59
1:C:14:ALA:HB3	1:C:15:PRO:HD3	1.84	0.58
1:C:103:GLN:OE1	1:C:717:HIS:HD2	1.86	0.58
1:C:495:ASP:O	1:C:499:ILE:HG13	2.03	0.58
1:D:387:GLN:O	1:D:391:GLU:HG3	2.03	0.58
1:D:159:PRO:HG3	1:D:402:THR:HG22	1.84	0.58
1:C:99:GLU:O	1:C:103:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:PRO:HG3	1:C:402:THR:HG22	1.86	0.57
1:D:23:LEU:HD22	1:D:27:LYS:HE3	1.86	0.57
1:B:159:PRO:CG	1:B:402:THR:HG22	2.35	0.57
1:D:10:LEU:HD13	1:D:39:THR:HB	1.86	0.57
1:C:148:PRO:HD3	1:C:565:MET:HA	1.86	0.57
1:A:236:ILE:HD13	1:A:270:ILE:HA	1.87	0.57
1:B:367:ASP:OD1	1:B:371:HIS:HE1	1.88	0.57
1:B:569:VAL:HB	1:B:577:LEU:HB3	1.86	0.57
1:B:665:LEU:O	1:B:669:GLN:HG3	2.04	0.57
1:D:149:LEU:HG	1:D:153:ASN:ND2	2.19	0.57
1:D:14:ALA:HB3	1:D:15:PRO:HD3	1.87	0.56
1:C:12:ASP:O	1:C:15:PRO:HD2	2.05	0.56
1:C:387:GLN:O	1:C:391:GLU:HG3	2.05	0.56
1:C:97:ILE:O	1:C:101:GLN:HG3	2.05	0.56
1:C:10:LEU:HD13	1:C:39:THR:HB	1.86	0.56
1:C:738:ALA:HB3	1:C:739:PRO:HD3	1.86	0.56
1:B:116:THR:OG1	1:B:119:GLU:HG3	2.06	0.56
1:C:665:LEU:O	1:C:669:GLN:HG3	2.05	0.56
1:D:149:LEU:HG	1:D:153:ASN:HD21	1.71	0.56
1:A:23:LEU:HD13	4:A:1166:HOH:O	2.06	0.55
1:C:622:LYS:O	1:C:624:PRO:HD3	2.06	0.55
1:A:23:LEU:HD22	1:A:27:LYS:HE3	1.88	0.55
1:B:573:SER:HB2	4:B:1014:HOH:O	2.05	0.55
1:B:13:GLU:HB3	1:B:590:VAL:HG21	1.87	0.55
1:A:267:PHE:CD2	1:A:344:PRO:HG3	2.42	0.55
1:D:15:PRO:HG3	1:D:601:TRP:CZ2	2.42	0.55
1:C:193:PRO:HG3	4:C:1015:HOH:O	2.07	0.55
1:D:697:LYS:O	1:D:701:GLU:HG3	2.07	0.55
1:A:241:GLU:HG2	4:A:1269:HOH:O	2.05	0.54
1:A:569:VAL:HB	1:A:577:LEU:HB3	1.89	0.54
1:B:15:PRO:HG3	1:B:601:TRP:CH2	2.42	0.54
1:B:313:LYS:HB2	1:B:313:LYS:NZ	2.21	0.54
1:A:111:PRO:O	1:A:123:LYS:HD2	2.06	0.54
1:D:236:ILE:HD13	1:D:270:ILE:HA	1.89	0.54
1:D:59:THR:HG23	4:D:1160:HOH:O	2.07	0.54
1:D:40:ARG:CZ	1:D:68:GLU:OE2	2.55	0.54
1:A:625:LYS:NZ	1:A:679:GLU:HB2	2.23	0.54
1:C:555:PRO:HB3	1:C:565:MET:CE	2.37	0.54
1:C:232:LEU:O	1:C:236:ILE:HG13	2.08	0.54
1:D:313:LYS:NZ	1:D:313:LYS:HB2	2.23	0.54
1:C:527:PHE:CZ	1:C:531:ARG:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:PRO:HG2	1:D:123:LYS:HB2	1.91	0.53
1:A:40:ARG:CZ	1:A:68:GLU:HG2	2.39	0.53
1:C:303:ARG:O	1:C:306:THR:HG22	2.08	0.53
1:D:44:LEU:C	1:D:44:LEU:HD13	2.29	0.53
1:D:297:ILE:HG22	1:D:342:HIS:HA	1.91	0.53
1:A:697:LYS:O	1:A:701:GLU:HG3	2.08	0.53
1:D:625:LYS:HZ1	1:D:679:GLU:HB2	1.73	0.53
1:C:54:GLU:HG2	1:C:55:TYR:CD1	2.44	0.52
1:A:499:ILE:O	1:A:503:GLU:HG3	2.10	0.52
1:C:90:VAL:HB	1:C:91:PRO:HD3	1.91	0.52
1:D:569:VAL:HB	1:D:577:LEU:HB3	1.90	0.52
1:A:387:GLN:O	1:A:391:GLU:HG3	2.09	0.52
1:B:111:PRO:HG2	1:B:123:LYS:HB2	1.92	0.52
1:B:297:ILE:HG22	1:B:342:HIS:HA	1.91	0.52
1:C:121:ASP:O	1:C:125:ARG:HG2	2.09	0.52
1:B:98:LYS:O	1:B:102:GLN:HG3	2.10	0.52
1:B:649:ARG:C	1:B:650:LYS:HD3	2.30	0.52
1:C:241:GLU:O	1:C:245:LYS:HG3	2.09	0.52
1:D:607:PHE:CE1	1:D:663:LEU:HD22	2.45	0.51
1:A:650:LYS:O	1:A:651:VAL:HG23	2.09	0.51
1:B:407:VAL:HG23	1:B:532:ILE:HD12	1.93	0.51
1:D:665:LEU:O	1:D:669:GLN:HG3	2.11	0.51
1:A:297:ILE:HG22	1:A:342:HIS:HA	1.93	0.50
1:D:148:PRO:HD3	1:D:565:MET:HA	1.92	0.50
1:C:436:ARG:HG2	1:C:447:GLU:HG3	1.92	0.50
1:C:632:THR:HG21	1:C:671:LEU:HD23	1.93	0.50
1:C:313:LYS:HB2	1:C:313:LYS:NZ	2.27	0.50
1:B:72:LEU:C	1:B:72:LEU:HD23	2.32	0.50
1:B:12:ASP:O	1:B:15:PRO:HD2	2.11	0.50
1:D:7:ILE:HG21	1:D:69:LEU:HD21	1.94	0.49
1:B:300:LEU:C	1:B:300:LEU:HD23	2.33	0.49
1:C:57:THR:OG1	1:C:60:GLN:HG3	2.12	0.49
1:C:149:LEU:HG	1:C:153:ASN:HD21	1.77	0.49
1:C:607:PHE:CD1	1:C:663:LEU:HD22	2.47	0.49
1:D:10:LEU:CD1	1:D:39:THR:HB	2.43	0.49
1:C:504:ARG:HD3	1:C:504:ARG:C	2.33	0.49
1:D:499:ILE:O	1:D:503:GLU:HG3	2.12	0.49
1:B:717:HIS:HE1	4:B:1010:HOH:O	1.95	0.49
1:A:625:LYS:HZ2	1:A:679:GLU:HB2	1.77	0.48
1:C:300:LEU:O	1:C:304:ILE:HG23	2.12	0.48
1:C:651:VAL:HG12	1:C:652:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:O	1:D:101:GLN:HG3	2.13	0.48
1:A:148:PRO:HG2	1:A:608:LEU:HD13	1.95	0.48
1:B:387:GLN:O	1:B:391:GLU:HG3	2.13	0.48
1:C:66:LEU:HD13	1:C:66:LEU:C	2.33	0.48
1:B:622:LYS:O	1:B:624:PRO:HD3	2.14	0.48
1:C:221:ILE:HD13	1:C:497:GLN:HB3	1.95	0.48
1:D:414:ALA:HB3	1:D:465:PRO:HB3	1.95	0.48
1:A:414:ALA:HB3	1:A:465:PRO:HB3	1.94	0.48
1:B:14:ALA:HB3	1:B:15:PRO:HD3	1.95	0.48
1:B:607:PHE:CE1	1:B:663:LEU:HD22	2.49	0.48
1:B:51:THR:C	1:B:53:PRO:HD3	2.34	0.48
1:B:313:LYS:HB2	1:B:313:LYS:HZ2	1.78	0.48
1:C:98:LYS:O	1:C:102:GLN:HG3	2.14	0.48
1:D:232:LEU:HD23	1:D:269:GLN:OE1	2.14	0.48
1:C:300:LEU:HD23	1:C:300:LEU:C	2.33	0.48
1:C:569:VAL:HB	1:C:577:LEU:HB3	1.96	0.48
1:D:15:PRO:HG3	1:D:601:TRP:CH2	2.49	0.48
1:D:573:SER:HB2	4:D:935:HOH:O	2.14	0.48
1:A:152:LYS:HE3	1:A:156:ARG:HH12	1.79	0.47
1:C:157:LYS:C	1:C:159:PRO:HD3	2.34	0.47
1:C:429:ILE:HG13	1:C:450:VAL:HB	1.96	0.47
1:D:51:THR:C	1:D:53:PRO:HD3	2.34	0.47
1:A:287:LYS:NZ	1:D:149:LEU:HD21	2.29	0.47
1:C:573:SER:HB2	4:C:945:HOH:O	2.13	0.47
1:C:529:LEU:O	1:C:532:ILE:HG22	2.14	0.47
1:D:340:ASN:HD22	1:D:340:ASN:C	2.18	0.47
1:A:148:PRO:HG3	1:A:566:LEU:HG	1.96	0.47
1:B:57:THR:OG1	1:B:60:GLN:HG3	2.15	0.47
1:D:40:ARG:HD3	1:D:40:ARG:HA	1.77	0.47
1:D:72:LEU:O	1:D:78:ALA:HB2	2.15	0.47
1:D:114:PRO:CG	1:D:123:LYS:HD2	2.45	0.47
1:B:738:ALA:HB3	1:B:739:PRO:HD3	1.97	0.47
1:C:72:LEU:C	1:C:72:LEU:HD23	2.36	0.47
1:C:445:LEU:N	1:C:445:LEU:HD12	2.30	0.47
1:A:199:GLU:HG2	1:A:209:VAL:HA	1.96	0.47
1:C:101:GLN:HA	1:C:105:TYR:O	2.15	0.47
1:D:353:MET:HB2	1:D:354:PRO:HD3	1.97	0.47
1:A:111:PRO:HG2	1:A:123:LYS:HB2	1.98	0.46
1:C:51:THR:C	1:C:53:PRO:HD3	2.35	0.46
1:A:125:ARG:HD3	4:A:844:HOH:O	2.15	0.46
1:B:118:THR:O	1:B:122:VAL:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:TYR:CE1	1:C:655:ASP:HB3	2.51	0.46
1:A:98:LYS:O	1:A:102:GLN:HG3	2.16	0.46
1:C:52:PHE:N	1:C:53:PRO:HD3	2.30	0.46
1:C:197:LYS:O	1:C:437:VAL:HA	2.15	0.46
1:C:469:TRP:CZ2	1:C:541:VAL:HG12	2.50	0.46
1:C:492:ARG:HB2	1:C:495:ASP:HB2	1.96	0.46
1:A:203:LYS:C	1:A:205:GLY:H	2.18	0.46
1:D:300:LEU:C	1:D:300:LEU:HD23	2.35	0.46
1:B:242:ASP:O	1:B:246:GLN:NE2	2.49	0.46
1:A:13:GLU:HB3	1:A:590:VAL:HG21	1.98	0.46
1:C:565:MET:HB3	1:C:565:MET:HE2	1.77	0.46
1:A:388:VAL:HG21	1:A:522:VAL:HG13	1.98	0.46
1:B:23:LEU:HB3	1:B:24:PRO:HD3	1.97	0.46
1:B:236:ILE:CD1	1:B:270:ILE:HG12	2.45	0.46
1:C:498:VAL:O	1:C:502:VAL:HG23	2.16	0.46
1:C:22:LEU:HB2	1:C:660:HIS:CE1	2.51	0.45
1:B:66:LEU:HD13	1:B:137:VAL:HG11	1.97	0.45
1:B:66:LEU:HD13	1:B:66:LEU:C	2.37	0.45
1:B:414:ALA:HB3	1:B:465:PRO:HB3	1.97	0.45
1:A:607:PHE:CE1	1:A:663:LEU:HD22	2.51	0.45
1:A:109:ASP:O	1:A:111:PRO:HD3	2.17	0.45
1:B:40:ARG:CZ	1:B:68:GLU:OE2	2.65	0.45
1:C:148:PRO:HG2	1:C:608:LEU:HD13	1.98	0.45
1:C:504:ARG:HD3	1:C:504:ARG:O	2.17	0.45
1:A:145:ARG:HD3	1:A:551:THR:HB	1.98	0.45
1:A:204:ASP:HB2	1:D:644:ASN:HB2	1.98	0.45
1:C:46:GLY:O	1:C:62:ILE:HD11	2.16	0.45
1:D:202:ALA:HB3	1:D:204:ASP:OD1	2.17	0.44
1:C:267:PHE:CD2	1:C:344:PRO:HG3	2.52	0.44
1:C:45:ALA:O	1:C:49:ILE:HG13	2.17	0.44
1:C:229:LYS:HG3	1:C:269:GLN:OE1	2.18	0.44
1:D:223:ASP:OD2	1:D:494:HIS:ND1	2.43	0.44
1:B:429:ILE:HA	1:B:430:PRO:HD3	1.74	0.44
1:B:499:ILE:O	1:B:503:GLU:HG3	2.18	0.44
1:B:504:ARG:NH2	4:B:1130:HOH:O	2.50	0.44
1:A:4:PRO:HD2	1:A:34:GLY:O	2.18	0.44
1:D:223:ASP:OD1	1:D:459:CYS:HB2	2.17	0.44
1:B:676:GLU:N	1:B:676:GLU:OE1	2.50	0.44
1:D:13:GLU:HB3	1:D:590:VAL:HG21	2.00	0.43
1:C:204:ASP:OD1	1:C:206:SER:HB2	2.18	0.43
1:B:90:VAL:HB	1:B:91:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLU:HB3	1:C:590:VAL:CG2	2.47	0.43
1:C:147:ALA:HA	1:C:565:MET:HB3	2.00	0.43
1:D:429:ILE:HA	1:D:430:PRO:HD3	1.69	0.43
1:C:40:ARG:CZ	1:C:68:GLU:OE2	2.67	0.43
1:B:384:GLY:O	1:B:388:VAL:HG23	2.18	0.43
1:C:677:ASP:OD1	1:C:679:GLU:HB2	2.18	0.43
1:D:598:TYR:CE1	1:D:655:ASP:HB3	2.54	0.43
1:B:157:LYS:C	1:B:159:PRO:HD3	2.39	0.43
1:D:77:ASP:OD1	1:D:621:TYR:OH	2.30	0.43
1:C:552:ASP:O	1:C:556:ILE:HG12	2.19	0.43
1:D:77:ASP:HB3	4:D:1364:HOH:O	2.19	0.43
1:A:672:ALA:O	1:A:681:GLN:HG3	2.18	0.42
1:C:428:GLN:HA	1:C:454:ASP:O	2.19	0.42
1:C:499:ILE:O	1:C:503:GLU:HG3	2.19	0.42
1:C:236:ILE:HD13	1:C:270:ILE:HA	2.02	0.42
1:C:617:LEU:C	1:C:617:LEU:HD23	2.40	0.42
1:D:625:LYS:NZ	1:D:679:GLU:HB2	2.35	0.42
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.84	0.42
1:C:384:GLY:O	1:C:388:VAL:HG23	2.20	0.42
1:C:407:VAL:HA	1:C:538:THR:O	2.19	0.42
1:D:159:PRO:HG2	1:D:402:THR:HG22	2.01	0.42
1:A:159:PRO:CG	1:A:402:THR:HG22	2.44	0.42
1:A:278:ALA:CB	1:A:319:ILE:HD13	2.50	0.42
1:B:114:PRO:CG	1:B:123:LYS:HD2	2.49	0.42
1:B:265:ILE:CG2	1:B:455:ILE:HD11	2.49	0.42
1:D:77:ASP:OD1	1:D:77:ASP:O	2.38	0.42
1:D:529:LEU:O	1:D:532:ILE:HG22	2.19	0.42
1:A:313:LYS:HB2	1:A:313:LYS:HZ2	1.83	0.42
1:A:464:ALA:O	1:A:572:MET:HE3	2.20	0.42
1:C:367:ASP:OD1	1:C:371:HIS:HE1	2.02	0.42
1:C:399:PHE:O	1:C:401:PRO:HD3	2.20	0.42
1:A:353:MET:HB2	1:A:354:PRO:HD3	2.01	0.42
1:C:166:SER:HG	1:C:168:ASP:CG	2.22	0.42
1:C:331:MET:SD	1:C:339:THR:HG22	2.59	0.42
1:D:300:LEU:O	1:D:304:ILE:HG23	2.20	0.42
1:B:52:PHE:N	1:B:53:PRO:HD3	2.35	0.41
1:A:573:SER:HB2	4:A:1254:HOH:O	2.19	0.41
1:B:60:GLN:HB3	1:B:105:TYR:CE2	2.55	0.41
1:B:478:ARG:CD	1:B:514:LEU:HD11	2.49	0.41
1:D:22:LEU:HB2	1:D:660:HIS:CE1	2.55	0.41
1:B:82:LYS:NZ	1:B:85:ASN:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:THR:O	1:B:120:LYS:HG3	2.20	0.41
1:C:149:LEU:HG	1:C:153:ASN:ND2	2.34	0.41
1:C:40:ARG:HA	1:C:40:ARG:HD3	1.94	0.41
1:C:340:ASN:HD22	1:C:340:ASN:C	2.23	0.41
1:C:349:VAL:HG13	1:C:350:ASP:N	2.36	0.41
1:C:353:MET:HB2	1:C:354:PRO:HD3	2.03	0.41
1:D:542:THR:HB	1:D:546:LEU:HB2	2.03	0.41
1:A:90:VAL:N	1:A:91:PRO:CD	2.83	0.41
1:C:223:ASP:O	1:C:458:MET:HA	2.20	0.41
1:C:265:ILE:CG2	1:C:455:ILE:HD11	2.51	0.41
1:C:245:LYS:HD2	4:C:981:HOH:O	2.20	0.41
1:C:446:LEU:HD12	1:C:446:LEU:N	2.36	0.41
1:C:487:TRP:HB2	1:C:542:THR:HG22	2.02	0.41
1:B:232:LEU:HD23	1:B:269:GLN:NE2	2.35	0.41
1:D:44:LEU:HD12	1:D:96:ALA:CB	2.50	0.41
1:A:223:ASP:O	1:A:458:MET:HA	2.21	0.41
1:B:4:PRO:HG2	4:B:1264:HOH:O	2.21	0.41
1:B:72:LEU:HD23	1:B:78:ALA:CB	2.51	0.41
1:B:147:ALA:HB2	1:B:559:LEU:HD11	2.03	0.41
1:B:148:PRO:HG3	1:B:566:LEU:HG	2.01	0.41
1:B:158:HIS:N	1:B:159:PRO:HD3	2.36	0.41
1:B:232:LEU:O	1:B:236:ILE:HG13	2.20	0.41
1:C:168:ASP:OD2	1:C:168:ASP:C	2.57	0.41
1:C:429:ILE:HA	1:C:430:PRO:HD3	1.75	0.41
1:D:5:LYS:HA	1:D:36:ALA:O	2.21	0.41
1:A:22:LEU:HB2	1:A:660:HIS:CE1	2.56	0.41
1:B:487:TRP:HB2	1:B:542:THR:HG22	2.03	0.41
1:C:567:SER:HB3	1:C:579:GLU:O	2.21	0.41
1:D:148:PRO:HG2	1:D:608:LEU:HD13	2.02	0.41
1:B:40:ARG:HA	1:B:40:ARG:HD3	1.96	0.40
1:B:109:ASP:O	1:B:111:PRO:HD3	2.20	0.40
1:C:93:LEU:O	1:C:97:ILE:HG13	2.21	0.40
1:A:147:ALA:HA	1:A:565:MET:CB	2.52	0.40
1:A:740:LEU:HD23	1:A:740:LEU:HA	1.87	0.40
1:B:145:ARG:HG2	1:B:567:SER:HA	2.02	0.40
1:B:416:LYS:HA	4:B:1198:HOH:O	2.20	0.40
1:B:600:ARG:CZ	1:B:649:ARG:NH1	2.84	0.40
1:C:223:ASP:OD2	1:C:494:HIS:ND1	2.54	0.40
1:A:456:TRP:CH2	1:A:458:MET:HB2	2.57	0.40
1:C:109:ASP:O	1:C:111:PRO:HD3	2.21	0.40
1:D:52:PHE:N	1:D:53:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:HB3	1:C:60:GLN:HB2	2.03	0.40
1:D:607:PHE:CD1	1:D:663:LEU:HD22	2.57	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	738/741 (100%)	717 (97%)	20 (3%)	1 (0%)	51 43
1	B	738/741 (100%)	715 (97%)	23 (3%)	0	100 100
1	C	737/741 (100%)	710 (96%)	26 (4%)	1 (0%)	51 43
1	D	738/741 (100%)	718 (97%)	20 (3%)	0	100 100
All	All	2951/2964 (100%)	2860 (97%)	89 (3%)	2 (0%)	51 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	ASP
1	C	204	ASP

### 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	600/601 (100%)	592 (99%)	8 (1%)	69	65
1	B	600/601 (100%)	589 (98%)	11 (2%)	59	53
1	C	600/601 (100%)	591 (98%)	9 (2%)	65	60
1	D	600/601 (100%)	592 (99%)	8 (1%)	69	65
All	All	2400/2404 (100%)	2364 (98%)	36 (2%)	65	60

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

Mol	Chain	Res	Type
1	A	23	LEU
1	A	44	LEU
1	A	66	LEU
1	A	178	ASN
1	A	223	ASP
1	A	340	ASN
1	A	649	ARG
1	A	676	GLU
1	B	10	LEU
1	B	44	LEU
1	B	223	ASP
1	B	246	GLN
1	B	326	ARG
1	B	340	ASN
1	B	504	ARG
1	B	589	HIS
1	B	649	ARG
1	B	650	LYS
1	B	676	GLU
1	C	23	LEU
1	C	44	LEU
1	C	340	ASN
1	C	356	MET
1	C	359	ASP
1	C	504	ARG
1	C	552	ASP
1	C	649	ARG
1	C	650	LYS
1	D	5	LYS
1	D	23	LEU
1	D	66	LEU
1	D	203	LYS
1	D	223	ASP

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Mol	Chain	Res	Type
1	D	326	ARG
1	D	340	ASN
1	D	676	GLU

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	178	ASN
1	A	217	GLN
1	A	325	GLN
1	A	635	GLN
1	A	669	GLN
1	B	85	ASN
1	B	234	ASN
1	B	246	GLN
1	B	269	GLN
1	B	371	HIS
1	B	395	GLN
1	B	396	HIS
1	B	635	GLN
1	B	683	GLN
1	B	717	HIS
1	C	153	ASN
1	C	158	HIS
1	C	234	ASN
1	C	320	GLN
1	C	371	HIS
1	C	395	GLN
1	C	635	GLN
1	C	681	GLN
1	C	717	HIS
1	D	102	GLN
1	D	135	ASN
1	D	178	ASN
1	D	217	GLN
1	D	325	GLN
1	D	591	GLN

### 5.3.3 RNA

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 9 ligands modelled in this entry, 5 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
3	ICT	B	744	2	12,12,12	1.97	5 (41%)	13,16,16	3.14	5 (38%)
3	ICT	D	743	2	12,12,12	1.87	5 (41%)	13,16,16	3.07	5 (38%)
3	ICT	A	743	2	12,12,12	1.96	5 (41%)	13,16,16	3.05	5 (38%)
3	ICT	C	743	2	12,12,12	1.83	4 (33%)	13,16,16	3.21	5 (38%)

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
3	ICT	B	744	2	-	0/16/16/16	-
3	ICT	D	743	2	-	1/16/16/16	-
3	ICT	A	743	2	-	2/16/16/16	-
3	ICT	C	743	2	-	0/16/16/16	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	744	ICT	O7-C2	3.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	743	ICT	O7-C2	3.31	1.48	1.42
3	D	743	ICT	O7-C2	3.26	1.48	1.42
3	A	743	ICT	C3-C2	-3.03	1.50	1.54
3	A	743	ICT	O7-C2	2.96	1.48	1.42
3	A	743	ICT	C4-C3	2.93	1.58	1.53
3	B	744	ICT	C4-C3	2.77	1.58	1.53
3	D	743	ICT	C4-C3	2.54	1.57	1.53
3	B	744	ICT	O6-C6	-2.45	1.22	1.30
3	D	743	ICT	C3-C2	-2.31	1.51	1.54
3	B	744	ICT	C3-C2	-2.25	1.51	1.54
3	C	743	ICT	C4-C3	2.18	1.57	1.53
3	C	743	ICT	O6-C6	-2.17	1.23	1.30
3	C	743	ICT	O1-C1	2.17	1.28	1.22
3	A	743	ICT	O6-C6	-2.14	1.23	1.30
3	A	743	ICT	O1-C1	2.14	1.28	1.22
3	B	744	ICT	O1-C1	2.11	1.28	1.22
3	D	743	ICT	O6-C6	-2.09	1.23	1.30
3	D	743	ICT	O1-C1	2.07	1.28	1.22

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	743	ICT	O6-C6-C3	7.06	133.47	114.03
3	B	744	ICT	O6-C6-C3	7.03	133.38	114.03
3	A	743	ICT	O6-C6-C3	6.88	132.98	114.03
3	D	743	ICT	O6-C6-C3	6.88	132.96	114.03
3	C	743	ICT	O7-C2-C1	-4.72	100.76	110.66
3	C	743	ICT	O5-C6-C3	-4.69	111.18	122.95
3	A	743	ICT	O5-C6-C3	-4.69	111.19	122.95
3	B	744	ICT	O5-C6-C3	-4.66	111.27	122.95
3	D	743	ICT	O5-C6-C3	-4.62	111.37	122.95
3	B	744	ICT	O7-C2-C1	-4.60	101.02	110.66
3	D	743	ICT	O7-C2-C1	-4.46	101.31	110.66
3	A	743	ICT	O7-C2-C1	-4.42	101.40	110.66
3	B	744	ICT	O6-C6-O5	-3.89	115.25	124.09
3	C	743	ICT	O6-C6-O5	-3.87	115.29	124.09
3	C	743	ICT	O7-C2-C3	3.82	119.86	110.58
3	D	743	ICT	O6-C6-O5	-3.77	115.54	124.09
3	A	743	ICT	O6-C6-O5	-3.71	115.66	124.09
3	B	744	ICT	O7-C2-C3	3.44	118.94	110.58
3	D	743	ICT	O7-C2-C3	3.16	118.27	110.58
3	A	743	ICT	O7-C2-C3	3.05	118.00	110.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	743	ICT	C4-C3-C6-O5
3	A	743	ICT	C4-C3-C6-O6
3	D	743	ICT	C4-C3-C6-O5

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.