



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:03 pm BST

PDB ID : 2CN2  
Title : Crystal Structures of Clostridium thermocellum Xyloglucanase  
Authors : Martinez-Fleites, C.; Taylor, E.J.; Guerreiro, C.I.; Prates, J.A.M.; Ferreira, L.M.A.; Fontes, C.M.G.A.; Baumann, M.J.; Brumer, H.; Davies, G.J.  
Deposited on : 2006-05-17  
Resolution : 2.10 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.

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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)  
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

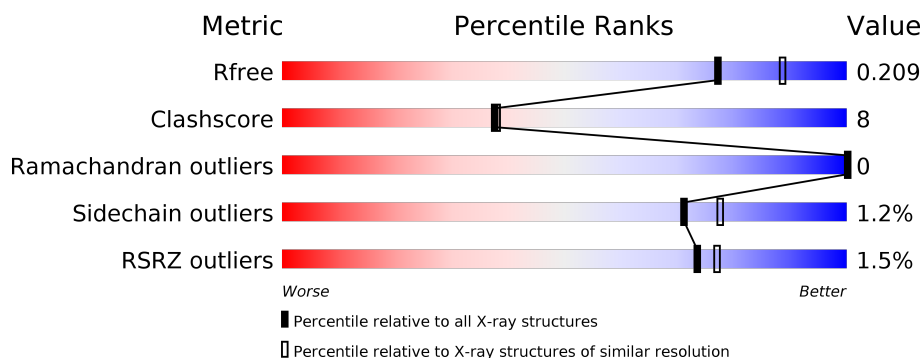
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	737	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	737	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </div> </div>
1	C	737	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• •</div> </div> </div>
1	D	737	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23900 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 BETA-1,4-XYLOGLUCAN HYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	704	Total	C	N	O	S	Se	0	1	0
			5450	3483	910	1033	5	19			
1	B	704	Total	C	N	O	S	Se	0	1	0
			5443	3479	908	1033	5	18			
1	C	704	Total	C	N	O	S	Se	0	0	0
			5448	3481	911	1033	5	18			
1	D	704	Total	C	N	O	S	Se	0	3	0
			5463	3493	911	1033	5	21			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cd	0	0
			3	3		
2	A	3	Total	Cd	0	0
			3	3		
2	D	5	Total	Cd	0	0
			5	5		
2	C	4	Total	Cd	0	0
			4	4		

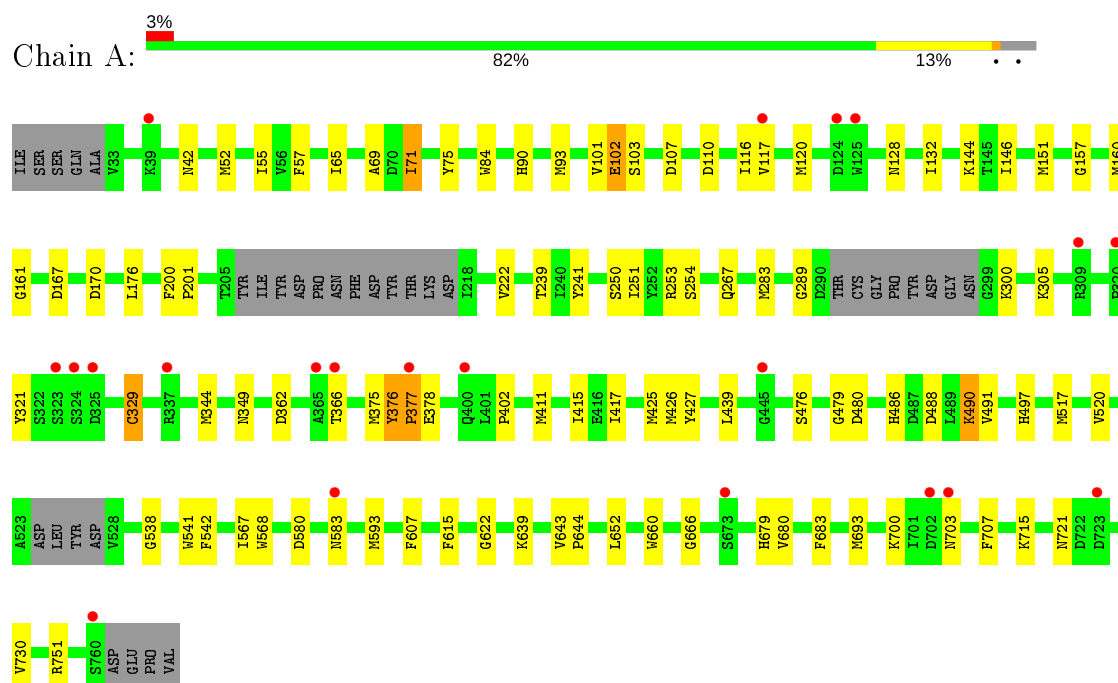
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	400	Total	O	0	0
			400	400		
3	B	550	Total	O	0	0
			550	550		
3	C	526	Total	O	0	0
			526	526		
3	D	605	Total	O	0	0
			605	605		

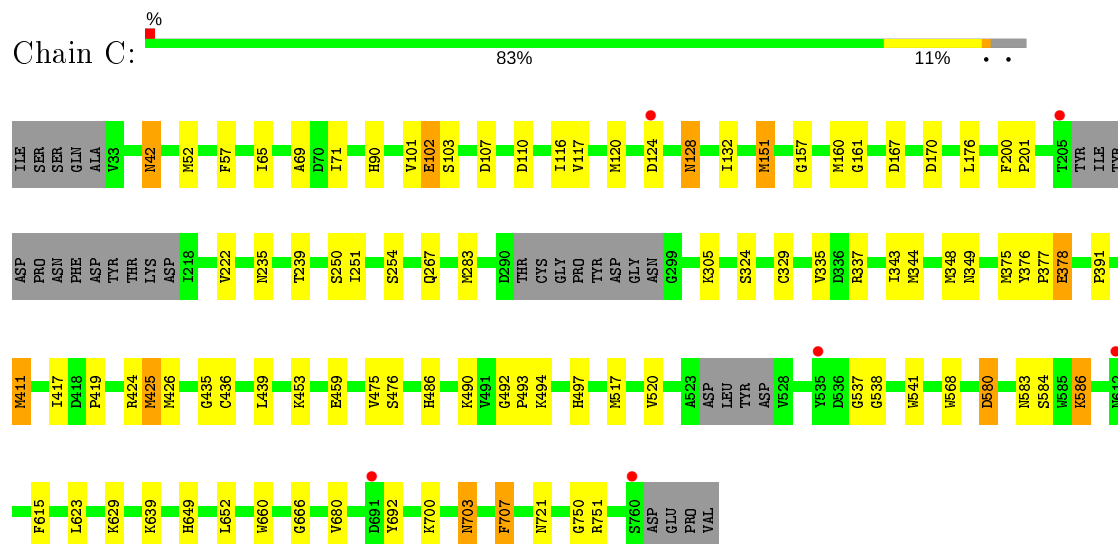
### 3 Residue-property plots [i](#)

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.

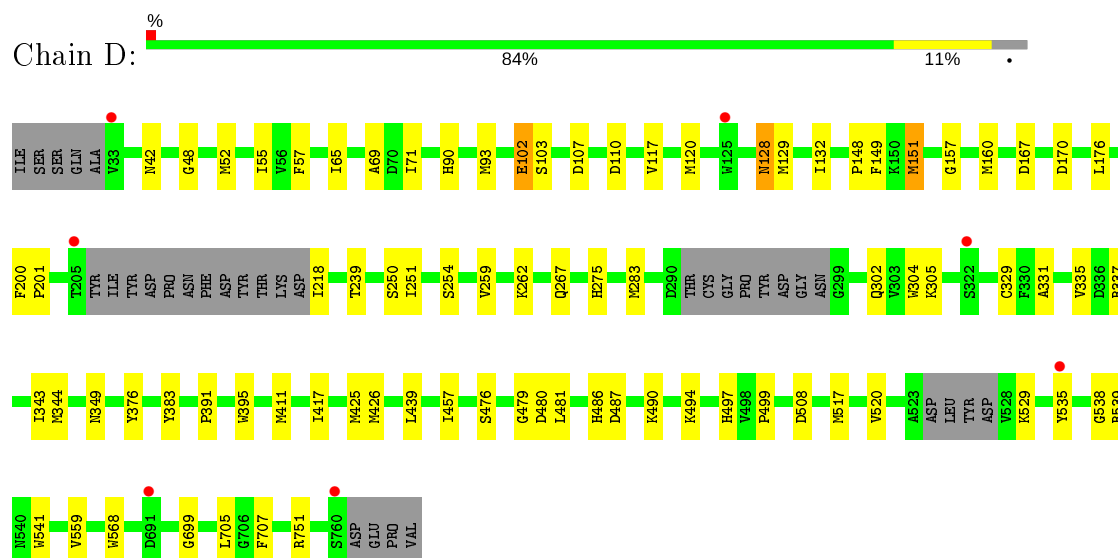
#### • Molecule 1: BETA-1,4-XYLOGLUCAN HYDROLASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.44Å 97.94Å 199.12Å 90.00° 97.62° 90.00°	Depositor
Resolution (Å)	19.90 – 2.10 19.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.90-2.10) 98.8 (19.90-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.210 0.176 , 0.209	Depositor DCC
$R_{free}$ test set	11183 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.45	0/5591	0.55	0/7590
1	B	0.53	1/5584 (0.0%)	0.58	1/7581 (0.0%)
1	C	0.60	3/5586 (0.1%)	0.60	0/7583
1	D	0.58	3/5610 (0.1%)	0.60	0/7613
All	All	0.55	7/22371 (0.0%)	0.58	1/30367 (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	4
1	C	0	3
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	378	GLU	CB-CG	-9.14	1.34	1.52
1	C	378	GLU	CG-CD	-6.54	1.42	1.51
1	B	376	TYR	CD1-CE1	-6.01	1.30	1.39
1	D	383	TYR	CD2-CE2	-5.29	1.31	1.39
1	C	329	CYS	CB-SG	-5.27	1.73	1.81
1	D	329	CYS	CB-SG	-5.11	1.73	1.81
1	D	376	TYR	CE1-CZ	-5.02	1.32	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	325	ASP	CB-CG-OD1	5.38	123.14	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	CYS	Peptide
1	A	376	TYR	Peptide
1	A	377	PRO	Peptide
1	A	71	ILE	Peptide
1	C	324	SER	Peptide
1	C	411	MSE	Mainchain
1	C	42	ASN	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	5450	0	5238	91	0
1	B	5443	0	5228	73	0
1	C	5448	0	5238	84	0
1	D	5463	0	5265	85	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
3	A	400	0	0	4	0
3	B	550	0	0	2	0
3	C	526	0	0	8	0
3	D	605	0	0	13	0
All	All	23900	0	20969	330	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 8.

All (330) 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:A:643:VAL:HG13	1:A:693:MSE:HE2	1.22	1.19
1:B:643:VAL:HG13	1:B:693:MSE:HE2	1.31	1.06
1:C:157:GLY:HA3	1:C:160:MSE:HE3	1.37	1.06
1:A:157:GLY:HA3	1:A:160:MSE:HE3	1.39	1.04
1:B:644:PRO:HD2	1:B:693:MSE:HE1	1.40	1.02
1:D:157:GLY:HA3	1:D:160:MSE:HE3	1.40	1.01
1:A:117:VAL:HG21	1:A:151:MSE:HE2	1.44	0.99
1:B:344:MSE:HE1	1:B:425:MSE:HG3	1.45	0.99
1:D:157:GLY:HA3	1:D:160:MSE:CE	1.93	0.98
1:A:344:MSE:HE1	1:A:425:MSE:HG3	1.46	0.96
1:B:117:VAL:HG22	1:B:151:MSE:HE3	1.46	0.95
1:D:344:MSE:HE1	1:D:425:MSE:HG3	1.48	0.95
1:C:117:VAL:CG2	1:C:151:MSE:HE2	1.97	0.94
1:A:102:GLU:HB3	1:A:117:VAL:HG13	1.48	0.93
1:B:643:VAL:HG13	1:B:693:MSE:CE	1.98	0.93
1:A:157:GLY:CA	1:A:160:MSE:HE3	2.00	0.91
1:C:344:MSE:HE1	1:C:425:MSE:HG3	1.53	0.91
1:A:644:PRO:HD2	1:A:693:MSE:HE1	1.54	0.90
1:A:93:MSE:HE1	1:A:679:HIS:NE2	1.86	0.90
1:C:157:GLY:CA	1:C:160:MSE:HE3	2.01	0.89
1:A:643:VAL:CG1	1:A:693:MSE:HE2	2.02	0.89
1:A:643:VAL:HG13	1:A:693:MSE:CE	2.03	0.89
1:B:117:VAL:HG23	1:B:132:ILE:HD13	1.56	0.88
1:C:102:GLU:HB3	1:C:117:VAL:HG13	1.57	0.87
1:C:425:MSE:HE2	1:C:436:CYS:SG	2.16	0.86
1:B:251:ILE:H	1:B:267:GLN:HE22	1.21	0.86
1:A:117:VAL:CG2	1:A:151:MSE:HE2	2.06	0.85
1:B:643:VAL:CG1	1:B:693:MSE:HE2	2.05	0.85
1:B:57:PHE:CZ	1:B:426:MSE:HE2	2.11	0.85
1:B:102:GLU:HB3	1:B:117:VAL:CG1	2.06	0.85
1:D:102:GLU:HB3	1:D:117:VAL:HG13	1.58	0.84
1:C:117:VAL:HG21	1:C:151:MSE:HE2	1.58	0.84
1:D:93:MSE:HE2	1:D:705:LEU:HD22	1.61	0.83
1:C:283:MSE:HE2	1:C:305:LYS:HD2	1.58	0.82
1:A:362:ASP:OD2	1:A:366:THR:HG22	1.79	0.81
1:C:517:MSE:HE2	1:C:538:GLY:CA	2.09	0.81
1:B:349:ASN:HD21	1:B:411[B]:MSE:H	1.27	0.81
1:B:349:ASN:HD21	1:B:411[A]:MSE:H	1.27	0.80
1:B:65:ILE:HG21	1:B:426:MSE:HE1	1.62	0.80
1:B:117:VAL:HG23	1:B:132:ILE:CD1	2.13	0.79
1:C:157:GLY:HA3	1:C:160:MSE:CE	2.12	0.79
1:C:517:MSE:HE2	1:C:538:GLY:N	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:PRO:HG2	1:C:494:LYS:HD3	1.66	0.78
1:D:157:GLY:CA	1:D:160:MSE:CE	2.61	0.78
1:C:349:ASN:HD21	1:C:411:MSE:H	1.31	0.77
1:D:517:MSE:HE2	1:D:538:GLY:CA	2.15	0.76
1:D:283:MSE:HE2	1:D:305:LYS:HD2	1.66	0.75
1:C:517:MSE:CE	1:C:538:GLY:HA3	2.16	0.75
1:C:65:ILE:HG21	1:C:426:MSE:HE1	1.69	0.74
1:D:117:VAL:HG21	1:D:151:MSE:HE2	1.69	0.74
1:A:65:ILE:HG21	1:A:426:MSE:HE1	1.68	0.73
1:A:151:MSE:CE	3:A:2103:HOH:O	2.36	0.73
1:C:490:LYS:HD2	3:C:2006:HOH:O	1.87	0.73
1:B:517:MSE:HE3	1:B:541:TRP:CH2	2.24	0.72
1:C:90:HIS:HD2	3:C:2052:HOH:O	1.72	0.72
1:C:517:MSE:CE	1:C:538:GLY:CA	2.67	0.72
1:D:129:MSE:HE3	1:D:149:PHE:N	2.04	0.71
1:D:157:GLY:CA	1:D:160:MSE:HE3	2.16	0.71
1:D:251:ILE:H	1:D:267:GLN:HE22	1.37	0.71
1:D:55:ILE:HG21	1:D:426:MSE:HE3	1.71	0.71
1:C:349:ASN:ND2	1:C:411:MSE:H	1.89	0.71
1:A:93:MSE:HE1	1:A:679:HIS:HE2	1.52	0.70
1:C:103:SER:HB3	1:C:117:VAL:HG12	1.74	0.70
1:D:90:HIS:HD2	3:D:2059:HOH:O	1.75	0.69
1:D:490:LYS:HD2	3:D:2009:HOH:O	1.93	0.69
1:C:151:MSE:CE	1:C:176:LEU:HD21	2.22	0.69
1:C:157:GLY:CA	1:C:160:MSE:CE	2.70	0.69
1:B:102:GLU:HB3	1:B:117:VAL:HG12	1.73	0.68
1:A:42:ASN:HD21	1:A:751:ARG:HH12	1.41	0.68
1:C:124:ASP:HB2	3:C:2092:HOH:O	1.95	0.67
1:A:57:PHE:CZ	1:A:426:MSE:HE2	2.29	0.67
1:A:376:TYR:HA	1:A:378:GLU:H	1.60	0.67
1:B:302:GLN:HE21	1:B:304:TRP:HE1	1.41	0.67
1:B:283:MSE:HE2	1:B:305:LYS:HD2	1.77	0.67
1:B:117:VAL:HG21	1:B:176:LEU:HD11	1.78	0.66
1:D:103:SER:HB3	1:D:117:VAL:HG12	1.78	0.66
1:B:117:VAL:HG21	1:B:176:LEU:CD1	2.26	0.66
1:B:349:ASN:ND2	1:B:411[B]:MSE:H	1.94	0.66
1:B:349:ASN:ND2	1:B:411[A]:MSE:H	1.94	0.66
1:D:117:VAL:CG2	1:D:151:MSE:HE2	2.25	0.65
1:D:157:GLY:CA	1:D:160:MSE:HE2	2.26	0.65
1:A:344:MSE:HE2	1:A:417:ILE:CG1	2.27	0.65
1:C:57:PHE:CZ	1:C:426:MSE:HE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:PHE:HB3	1:B:693:MSE:HE3	1.80	0.64
1:D:129:MSE:CE	1:D:148:PRO:C	2.66	0.64
1:C:151:MSE:HE1	1:C:176:LEU:HD21	1.79	0.64
1:C:517:MSE:HE1	1:C:538:GLY:HA3	1.80	0.63
1:D:218:ILE:N	3:D:2204:HOH:O	2.32	0.63
1:A:157:GLY:HA3	1:A:160:MSE:CE	2.24	0.63
1:A:55:ILE:HG21	1:A:426:MSE:HE3	1.80	0.63
1:B:42:ASN:HD21	1:B:751:ARG:HH12	1.45	0.63
1:B:302:GLN:NE2	1:B:304:TRP:HE1	1.96	0.63
1:C:251:ILE:H	1:C:267:GLN:HE22	1.47	0.62
1:B:102:GLU:HB3	1:B:117:VAL:HG13	1.80	0.62
1:B:93:MSE:HE1	1:B:679:HIS:NE2	2.15	0.62
1:A:349:ASN:HD21	1:A:411[B]:MSE:H	1.46	0.61
1:A:580:ASP:O	1:A:583:ASN:ND2	2.34	0.60
1:B:517:MSE:CE	1:B:541:TRP:CZ2	2.84	0.60
1:D:157:GLY:HA2	1:D:160:MSE:HE2	1.82	0.60
1:D:490:LYS:HD3	3:D:2008:HOH:O	2.01	0.60
1:C:90:HIS:CD2	3:C:2052:HOH:O	2.52	0.59
1:A:349:ASN:HD21	1:A:411[A]:MSE:H	1.47	0.59
1:C:344:MSE:HE2	1:C:417:ILE:CG1	2.32	0.59
1:A:517:MSE:HE3	1:A:541:TRP:CH2	2.37	0.58
1:A:251:ILE:H	1:A:267:GLN:HE22	1.50	0.58
1:B:57:PHE:HZ	1:B:426:MSE:HE2	1.67	0.58
1:D:250:SER:H	1:D:267:GLN:HE22	1.52	0.58
1:C:103:SER:HB3	1:C:117:VAL:CG1	2.33	0.58
1:C:476:SER:OG	1:C:486:HIS:HE1	1.86	0.58
1:D:167:ASP:HB3	1:D:170:ASP:O	2.04	0.58
1:A:375:MSE:O	1:A:378:GLU:HB3	2.04	0.58
1:D:250:SER:H	1:D:267:GLN:NE2	2.02	0.58
1:D:55:ILE:HG21	1:D:426:MSE:CE	2.34	0.57
1:D:479:GLY:O	1:D:480:ASP:HB2	2.05	0.57
1:D:517:MSE:HE2	1:D:538:GLY:N	2.19	0.57
1:D:117:VAL:HG22	1:D:151:MSE:HG2	1.87	0.56
1:A:157:GLY:CA	1:A:160:MSE:CE	2.80	0.56
1:D:517:MSE:CE	1:D:538:GLY:CA	2.83	0.56
1:A:117:VAL:HG13	1:A:117:VAL:O	2.05	0.56
1:B:71:ILE:HA	1:B:120:MSE:HE2	1.89	0.55
1:A:93:MSE:HE1	1:A:679:HIS:CD2	2.40	0.55
1:D:132:ILE:HD11	1:D:176:LEU:HD22	1.87	0.55
1:D:425:MSE:HB2	1:D:439:LEU:HD22	1.87	0.55
1:A:490:LYS:HE3	3:C:2101:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:HIS:HD2	3:A:2035:HOH:O	1.90	0.55
1:B:479:GLY:O	1:B:480:ASP:HB2	2.06	0.55
1:D:42:ASN:HD21	1:D:751:ARG:HH12	1.54	0.55
1:C:117:VAL:HG21	1:C:176:LEU:HD11	1.88	0.55
1:B:144:LYS:HE3	1:B:146:ILE:HD11	1.89	0.54
1:C:101:VAL:HG13	1:C:116:ILE:HG23	1.89	0.54
1:A:151:MSE:HE3	3:A:2103:HOH:O	2.03	0.54
1:D:151:MSE:CE	1:D:176:LEU:HD21	2.37	0.54
1:C:700:LYS:HE2	1:C:703:ASN:HA	1.89	0.54
1:A:683:PHE:HB3	1:A:693:MSE:HE3	1.89	0.54
1:B:57:PHE:CE2	1:B:426:MSE:HE2	2.43	0.54
1:C:117:VAL:HG22	1:C:151:MSE:HG2	1.90	0.54
1:B:344:MSE:HE2	1:B:417:ILE:CG1	2.38	0.53
1:B:344:MSE:HE2	1:B:417:ILE:HG13	1.90	0.53
1:C:517:MSE:HE2	1:C:537:GLY:C	2.27	0.53
1:D:90:HIS:CD2	3:D:2059:HOH:O	2.57	0.53
1:C:337:ARG:O	1:C:337:ARG:HG2	2.08	0.53
1:D:128:ASN:H	1:D:128:ASN:ND2	2.06	0.53
1:B:55:ILE:HG21	1:B:426:MSE:HE3	1.89	0.53
1:D:517:MSE:SE	3:D:2415:HOH:O	2.76	0.53
1:D:344:MSE:HE2	1:D:417:ILE:CG1	2.39	0.53
1:C:580:ASP:HB3	1:C:583:ASN:H	1.74	0.52
1:D:57:PHE:CE2	1:D:426:MSE:HE2	2.43	0.52
1:C:376:TYR:CG	1:C:377:PRO:HA	2.45	0.52
1:D:337:ARG:HD3	3:D:2026:HOH:O	2.09	0.52
1:D:517:MSE:HE3	1:D:541:TRP:CH2	2.43	0.52
1:A:132:ILE:HD11	1:A:176:LEU:HD22	1.91	0.52
1:B:101:VAL:HG13	1:B:116:ILE:HG23	1.90	0.52
1:B:57:PHE:CE2	1:B:426:MSE:CE	2.92	0.52
1:A:250:SER:H	1:A:267:GLN:HE22	1.57	0.52
1:A:349:ASN:ND2	1:A:411[B]:MSE:H	2.06	0.52
1:B:57:PHE:CZ	1:B:426:MSE:CE	2.90	0.52
1:C:425:MSE:CE	1:C:436:CYS:SG	2.93	0.52
1:A:117:VAL:HG22	1:A:151:MSE:HG3	1.92	0.52
1:A:349:ASN:ND2	1:A:411[A]:MSE:H	2.07	0.52
1:A:425:MSE:HB2	1:A:439:LEU:HD22	1.92	0.52
1:A:250:SER:H	1:A:267:GLN:NE2	2.07	0.52
1:C:580:ASP:OD2	1:C:584:SER:OG	2.27	0.52
1:D:151:MSE:HE3	3:D:2162:HOH:O	2.09	0.52
1:D:476:SER:O	1:D:497:HIS:HE1	1.91	0.52
1:D:349:ASN:HD21	1:D:411[B]:MSE:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HD11	1:C:176:LEU:HD22	1.91	0.51
1:D:349:ASN:HD21	1:D:411[A]:MSE:H	1.58	0.51
1:A:517:MSE:HE2	1:A:538:GLY:CA	2.40	0.51
1:C:128:ASN:ND2	1:C:128:ASN:H	2.08	0.51
1:D:508:ASP:HB3	1:D:559:VAL:HG23	1.92	0.51
1:B:517:MSE:CE	1:B:541:TRP:CH2	2.94	0.51
1:A:144:LYS:HE2	1:A:146:ILE:HD11	1.92	0.51
1:A:376:TYR:HA	1:A:378:GLU:N	2.26	0.51
1:C:42:ASN:HD21	1:C:751:ARG:HH12	1.59	0.50
1:D:129:MSE:HE3	1:D:148:PRO:C	2.28	0.50
1:B:250:SER:H	1:B:267:GLN:NE2	2.08	0.50
1:C:337:ARG:NE	1:C:419:PRO:O	2.43	0.50
1:D:391:PRO:HG2	1:D:494:LYS:HD3	1.94	0.50
1:D:128:ASN:H	1:D:128:ASN:HD22	1.59	0.50
1:B:117:VAL:HG22	1:B:151:MSE:CE	2.30	0.50
1:D:71:ILE:HA	1:D:120:MSE:HE2	1.94	0.50
1:A:700:LYS:HE2	1:A:703:ASN:HA	1.93	0.49
1:C:250:SER:H	1:C:267:GLN:HE22	1.59	0.49
1:C:639:LYS:HG3	1:C:680:VAL:HG12	1.94	0.49
1:D:517:MSE:CE	1:D:538:GLY:HA3	2.42	0.49
1:A:344:MSE:HE2	1:A:417:ILE:HD11	1.94	0.49
1:A:101:VAL:HG13	1:A:116:ILE:HG23	1.95	0.49
1:C:335:VAL:HG22	1:C:343:ILE:HG22	1.95	0.49
1:A:103:SER:HB3	1:A:117:VAL:HG12	1.93	0.49
1:A:283:MSE:HE2	1:A:305:LYS:HD2	1.94	0.49
1:D:129:MSE:CE	1:D:149:PHE:N	2.74	0.49
1:C:167:ASP:HB3	1:C:170:ASP:O	2.13	0.49
1:D:337:ARG:CD	3:D:2026:HOH:O	2.61	0.49
1:B:90:HIS:CD2	3:B:2057:HOH:O	2.66	0.49
1:C:707:PHE:CD2	1:C:721:ASN:HB3	2.47	0.48
1:B:128:ASN:H	1:B:128:ASN:HD22	1.61	0.48
1:B:279:ALA:HB1	1:B:340:PRO:HB3	1.95	0.48
1:D:117:VAL:HG23	1:D:132:ILE:HD13	1.94	0.48
1:A:71:ILE:HA	1:A:120:MSE:HE2	1.95	0.48
1:D:535:TYR:HE1	3:D:2460:HOH:O	1.96	0.48
1:C:250:SER:H	1:C:267:GLN:NE2	2.12	0.48
1:C:128:ASN:H	1:C:128:ASN:HD22	1.62	0.48
1:C:107:ASP:HB3	1:C:110:ASP:O	2.14	0.47
1:A:476:SER:OG	1:A:486:HIS:HE1	1.97	0.47
1:A:52:MSE:SE	1:A:69:ALA:HB2	2.64	0.47
1:B:251:ILE:H	1:B:267:GLN:NE2	2.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:MSE:HE3	1:D:541:TRP:CZ2	2.49	0.47
1:A:289:GLY:HA3	1:A:329:CYS:HB3	1.96	0.47
1:D:107:ASP:HB3	1:D:110:ASP:O	2.13	0.47
1:D:349:ASN:ND2	1:D:411[B]:MSE:H	2.12	0.47
1:D:487:ASP:OD2	1:D:539:ARG:NH2	2.44	0.47
1:A:517:MSE:CE	1:A:541:TRP:CZ2	2.97	0.47
1:B:683:PHE:CB	1:B:693:MSE:HE3	2.43	0.47
1:D:349:ASN:ND2	1:D:411[A]:MSE:H	2.12	0.47
1:B:517:MSE:HE3	1:B:541:TRP:HH2	1.75	0.47
1:A:102:GLU:HB3	1:A:117:VAL:CG1	2.32	0.47
1:B:128:ASN:ND2	1:B:128:ASN:H	2.13	0.47
1:C:580:ASP:OD1	1:C:583:ASN:HB2	2.15	0.47
1:D:395:TRP:O	1:D:499:PRO:HB3	2.14	0.47
1:D:476:SER:OG	1:D:486:HIS:HE1	1.97	0.47
1:A:377:PRO:O	1:A:402:PRO:HB3	2.14	0.46
1:A:476:SER:O	1:A:497:HIS:HE1	1.98	0.46
1:A:683:PHE:CB	1:A:693:MSE:HE3	2.45	0.46
1:B:132:ILE:HD11	1:B:176:LEU:HD22	1.98	0.46
1:B:511:GLU:OE1	1:B:601:ARG:HD3	2.16	0.46
1:C:157:GLY:HA2	1:C:160:MSE:CE	2.44	0.46
1:B:90:HIS:HD2	3:B:2057:HOH:O	1.97	0.46
1:C:476:SER:O	1:C:497:HIS:HE1	1.99	0.46
1:C:71:ILE:HA	1:C:120:MSE:HE2	1.96	0.46
1:C:424:ARG:NH2	3:C:2333:HOH:O	2.44	0.46
1:C:52:MSE:SE	1:C:69:ALA:HB2	2.66	0.46
1:C:239:THR:HA	1:C:254:SER:O	2.16	0.45
1:D:517:MSE:HE2	1:D:538:GLY:HA2	1.95	0.45
1:B:175:TYR:CZ	1:B:186:ARG:HD3	2.51	0.45
1:A:117:VAL:CG2	1:A:151:MSE:CE	2.89	0.45
1:C:517:MSE:HE3	1:C:541:TRP:CH2	2.52	0.45
1:A:490:LYS:HD2	1:A:490:LYS:HA	1.71	0.45
1:C:649:HIS:HD2	1:C:692:TYR:OH	2.00	0.45
1:D:149:PHE:HE1	1:D:151:MSE:HE1	1.82	0.45
1:B:649:HIS:HD2	1:B:692:TYR:OH	1.98	0.44
1:C:475:VAL:HG11	1:C:517:MSE:HE1	1.99	0.44
1:A:520:VAL:HG11	1:A:568:TRP:CD1	2.53	0.44
1:D:103:SER:CB	1:D:117:VAL:HG12	2.47	0.44
1:A:344:MSE:HE2	1:A:417:ILE:HG13	1.98	0.44
1:A:479:GLY:O	1:A:480:ASP:HB2	2.17	0.44
1:C:283:MSE:HE2	1:C:305:LYS:CD	2.37	0.44
1:C:615:PHE:CE2	1:C:666:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:HA	1:A:254:SER:O	2.18	0.44
1:A:488:ASP:HB3	1:A:491:VAL:HB	1.98	0.44
1:C:425:MSE:O	1:C:425:MSE:HE3	2.18	0.44
1:A:167:ASP:HB3	1:A:170:ASP:O	2.18	0.44
1:A:707:PHE:CD2	1:A:721:ASN:HB3	2.52	0.44
1:D:151:MSE:HE2	1:D:176:LEU:HD21	1.99	0.44
1:A:107:ASP:HB3	1:A:110:ASP:O	2.18	0.43
1:B:520:VAL:HG11	1:B:568:TRP:CD1	2.52	0.43
1:D:65:ILE:HG21	1:D:426:MSE:HE1	2.00	0.43
1:D:200:PHE:HA	1:D:201:PRO:HD3	1.85	0.43
1:A:75:TYR:HB3	1:A:84:TRP:HB3	1.99	0.43
1:C:520:VAL:HG11	1:C:568:TRP:CD1	2.53	0.43
1:A:344:MSE:HE2	1:A:417:ILE:CD1	2.48	0.43
1:C:349:ASN:HD21	1:C:411:MSE:N	2.07	0.43
1:A:128:ASN:H	1:A:128:ASN:ND2	2.16	0.43
1:D:117:VAL:HG22	1:D:151:MSE:CG	2.49	0.43
1:D:497:HIS:HD2	3:D:2426:HOH:O	2.02	0.43
1:A:517:MSE:HE3	1:A:541:TRP:CZ2	2.54	0.43
1:B:707:PHE:CD2	1:B:721:ASN:HB3	2.54	0.43
1:C:425:MSE:HB2	1:C:439:LEU:HD22	2.00	0.43
1:D:93:MSE:HE3	3:D:2552:HOH:O	2.18	0.43
1:B:117:VAL:HG21	1:B:176:LEU:HD13	1.99	0.43
1:B:118:ALA:O	1:B:151:MSE:HE2	2.19	0.43
1:B:376:TYR:HA	1:B:377:PRO:HA	1.65	0.43
1:B:606:LYS:HA	1:B:618:SER:O	2.19	0.43
1:D:117:VAL:HG21	1:D:176:LEU:HD11	2.00	0.43
1:D:335:VAL:HG22	1:D:343:ILE:HG22	2.00	0.42
1:A:567:ILE:HD12	1:A:607:PHE:CD1	2.54	0.42
1:C:103:SER:CB	1:C:117:VAL:HG12	2.47	0.42
1:D:520:VAL:HG11	1:D:568:TRP:CD1	2.54	0.42
1:A:567:ILE:HD11	1:A:622:GLY:HA3	2.01	0.42
1:D:302:GLN:NE2	1:D:304:TRP:HE1	2.18	0.42
1:A:300:LYS:HB3	1:A:321:TYR:CE1	2.54	0.42
1:D:52:MSE:SE	1:D:69:ALA:HB2	2.70	0.42
1:A:593:MSE:HB3	1:A:593:MSE:HE2	1.94	0.42
1:A:615:PHE:CE2	1:A:666:GLY:HA3	2.53	0.42
1:B:583:ASN:HD21	1:C:124:ASP:HB3	1.85	0.42
1:A:542:PHE:CD2	1:D:129:MSE:HE2	2.55	0.42
1:A:344:MSE:HE1	1:A:425:MSE:CG	2.34	0.42
1:A:652:LEU:HB2	1:A:660:TRP:HB2	2.02	0.42
1:D:239:THR:HA	1:D:254:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLY:HA2	1:C:222:VAL:O	2.20	0.42
1:C:435:GLY:HA3	1:C:453:LYS:HG3	2.02	0.42
1:C:459:GLU:HA	1:C:750:GLY:O	2.19	0.42
1:D:251:ILE:H	1:D:267:GLN:NE2	2.09	0.42
1:A:486:HIS:HD2	3:A:2006:HOH:O	2.02	0.41
1:C:235:ASN:HB3	1:D:259:VAL:HG11	2.00	0.41
1:A:490:LYS:CE	3:C:2101:HOH:O	2.66	0.41
1:B:52:MSE:SE	1:B:69:ALA:HB2	2.70	0.41
1:D:411[A]:MSE:HE1	3:D:2064:HOH:O	2.20	0.41
1:A:157:GLY:HA2	1:A:160:MSE:CE	2.50	0.41
1:A:157:GLY:HA2	1:A:160:MSE:HE3	1.96	0.41
1:B:476:SER:O	1:B:497:HIS:HE1	2.04	0.41
1:B:529:LYS:HG3	1:B:547:GLU:HG3	2.03	0.41
1:A:707:PHE:HE1	1:A:730:VAL:HG21	1.86	0.41
1:C:200:PHE:HA	1:C:201:PRO:HD3	1.85	0.41
1:A:415:ILE:HG13	1:A:427:TYR:HB3	2.03	0.41
1:B:492:GLY:HA2	1:B:493:PRO:HD3	1.97	0.41
1:C:117:VAL:HG22	1:C:151:MSE:CG	2.49	0.41
1:A:241:TYR:CE1	1:A:253:ARG:HD3	2.55	0.41
1:D:48:GLY:HA2	1:D:457:ILE:HG22	2.02	0.41
1:D:275:HIS:HD2	1:D:331:ALA:O	2.04	0.41
1:B:200:PHE:HA	1:B:201:PRO:HD3	1.97	0.41
1:C:586:LYS:NZ	3:C:2427:HOH:O	2.53	0.41
1:C:652:LEU:HB2	1:C:660:TRP:HB2	2.03	0.41
1:A:161:GLY:HA2	1:A:222:VAL:O	2.21	0.40
1:B:137:ASP:O	1:B:138:ARG:HB2	2.22	0.40
1:B:180:CYS:HA	1:B:218:ILE:HB	2.03	0.40
1:B:462:VAL:HB	1:B:747:ALA:HB1	2.03	0.40
1:D:517:MSE:HE1	1:D:538:GLY:HA3	2.03	0.40
1:C:344:MSE:HE2	1:C:417:ILE:HD11	2.03	0.40
1:C:492:GLY:HA2	1:C:493:PRO:HD3	1.95	0.40
1:D:93:MSE:HE1	1:D:699:GLY:HA2	2.03	0.40
1:A:639:LYS:HG3	1:A:680:VAL:HG12	2.02	0.40
1:B:707:PHE:N	1:B:707:PHE:CD1	2.88	0.40
1:C:586:LYS:HE3	1:C:623:LEU:HD22	2.03	0.40
1:A:200:PHE:HA	1:A:201:PRO:HD3	1.87	0.40
1:B:250:SER:H	1:B:267:GLN:HE22	1.68	0.40
1:C:117:VAL:HG23	1:C:132:ILE:HD13	2.02	0.40
1:C:348:MSE:HA	1:C:349:ASN:HA	1.82	0.40
1:B:376:TYR:CG	1:B:377:PRO:HA	2.56	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	697/737 (95%)	675 (97%)	22 (3%)	0	100	100
1	B	697/737 (95%)	677 (97%)	20 (3%)	0	100	100
1	C	696/737 (94%)	673 (97%)	23 (3%)	0	100	100
1	D	699/737 (95%)	678 (97%)	21 (3%)	0	100	100
All	All	2789/2948 (95%)	2703 (97%)	86 (3%)	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	573/585 (98%)	570 (100%)	3 (0%)	88	92
1	B	572/585 (98%)	565 (99%)	7 (1%)	71	77
1	C	573/585 (98%)	562 (98%)	11 (2%)	57	63
1	D	576/585 (98%)	569 (99%)	7 (1%)	71	77
All	All	2294/2340 (98%)	2266 (99%)	28 (1%)	71	77

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	A	490	LYS

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Mol	Chain	Res	Type
1	A	715	LYS
1	B	102	GLU
1	B	117	VAL
1	B	128	ASN
1	B	148	PRO
1	B	151	MSE
1	B	583	ASN
1	B	707	PHE
1	C	102	GLU
1	C	128	ASN
1	C	151	MSE
1	C	375	MSE
1	C	378	GLU
1	C	425	MSE
1	C	580	ASP
1	C	586	LYS
1	C	629	LYS
1	C	703	ASN
1	C	707	PHE
1	D	102	GLU
1	D	128	ASN
1	D	151	MSE
1	D	262	LYS
1	D	481	LEU
1	D	529	LYS
1	D	707	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	90	HIS
1	A	128	ASN
1	A	169	ASN
1	A	267	GLN
1	A	349	ASN
1	A	382	HIS
1	A	486	HIS
1	A	497	HIS
1	A	590	ASN
1	B	42	ASN
1	B	90	HIS

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Mol	Chain	Res	Type
1	B	128	ASN
1	B	169	ASN
1	B	267	GLN
1	B	302	GLN
1	B	349	ASN
1	B	497	HIS
1	B	583	ASN
1	B	590	ASN
1	B	649	HIS
1	C	42	ASN
1	C	90	HIS
1	C	128	ASN
1	C	169	ASN
1	C	267	GLN
1	C	302	GLN
1	C	349	ASN
1	C	486	HIS
1	C	497	HIS
1	C	581	ASN
1	C	590	ASN
1	C	649	HIS
1	D	42	ASN
1	D	90	HIS
1	D	128	ASN
1	D	267	GLN
1	D	302	GLN
1	D	349	ASN
1	D	486	HIS
1	D	497	HIS
1	D	590	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	686/737 (93%)	-0.07	21 (3%) 49 55	11, 23, 36, 48	0
1	B	686/737 (93%)	-0.35	6 (0%) 84 86	8, 17, 28, 34	1 (0%)
1	C	686/737 (93%)	-0.32	6 (0%) 84 86	9, 17, 28, 35	0
1	D	686/737 (93%)	-0.41	7 (1%) 82 85	8, 14, 24, 35	0
All	All	2744/2948 (93%)	-0.29	40 (1%) 73 77	8, 17, 31, 48	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	760	SER	6.6
1	A	760	SER	5.1
1	D	760	SER	5.0
1	A	309	ARG	4.2
1	A	125	TRP	4.0
1	B	125	TRP	4.0
1	D	125	TRP	4.0
1	C	205	THR	3.9
1	C	535	TYR	3.8
1	D	535	TYR	3.8
1	A	124	ASP	3.6
1	A	703	ASN	3.4
1	A	365	ALA	3.3
1	A	400	GLN	3.2
1	A	324	SER	3.0
1	A	366	THR	2.9
1	A	323	SER	2.9
1	B	124	ASP	2.7
1	D	205	THR	2.7
1	B	760	SER	2.7
1	D	691	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	703	ASN	2.6
1	A	117	VAL	2.5
1	C	691	ASP	2.5
1	D	322	SER	2.5
1	B	702	ASP	2.4
1	A	723	ASP	2.3
1	A	377	PRO	2.3
1	A	702	ASP	2.3
1	C	124	ASP	2.3
1	D	33	VAL	2.3
1	C	612	ASN	2.3
1	A	325	ASP	2.2
1	A	673	SER	2.2
1	A	320	PRO	2.2
1	B	586	LYS	2.2
1	A	583	ASN	2.1
1	A	337	ARG	2.1
1	A	445	GLY	2.1
1	A	39	LYS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CD	A	1763	1/1	0.89	0.08	80,80,80,80	0
2	CD	C	1762	1/1	0.93	0.08	64,64,64,64	0
2	CD	C	1764	1/1	0.95	0.06	79,79,79,79	0
2	CD	D	1764	1/1	0.96	0.05	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CD	D	1763	1/1	0.97	0.08	50,50,50,50	0
2	CD	B	1763	1/1	0.98	0.12	52,52,52,52	0
2	CD	C	1763	1/1	0.98	0.06	69,69,69,69	0
2	CD	D	1765	1/1	0.98	0.09	50,50,50,50	0
2	CD	D	1761	1/1	0.99	0.03	43,43,43,43	0
2	CD	A	1761	1/1	0.99	0.02	28,28,28,28	0
2	CD	C	1761	1/1	1.00	0.02	22,22,22,22	0
2	CD	A	1762	1/1	1.00	0.04	21,21,21,21	0
2	CD	B	1761	1/1	1.00	0.02	20,20,20,20	0
2	CD	D	1762	1/1	1.00	0.02	21,21,21,21	0
2	CD	B	1762	1/1	1.00	0.04	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.