



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:41 AM GMT

PDB ID : 1V3J  
Title : Crystal structure of F283L mutant cyclodextrin glycosyltransferase  
Authors : Kanai, R.; Haga, K.; Akiba, T.; Yamane, K.; Harata, K.  
Deposited on : 2003-11-03  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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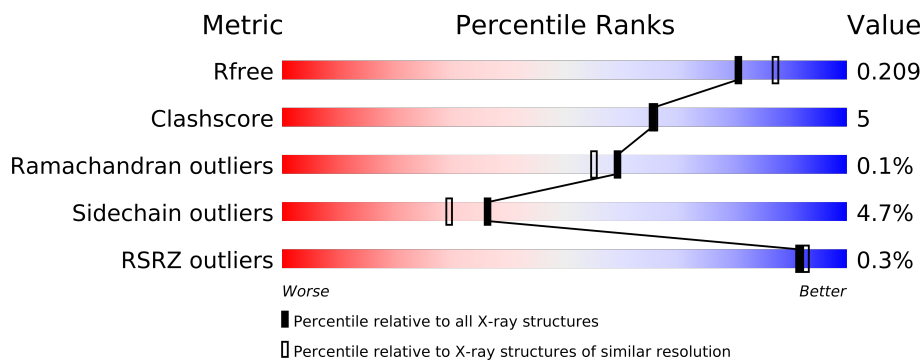
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	686	
1	B	686	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11226 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cyclomaltodextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5309	3351	906	1036	16			
1	B	686	Total	C	N	O	S	0	0	0
			5309	3351	906	1036	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LEU	PHE	ENGINEERED	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	283	LEU	PHE	ENGINEERED	UNP P05618
B	452	PRO	ARG	SEE REMARK 999	UNP P05618
B	454	GLY	ALA	SEE REMARK 999	UNP P05618

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

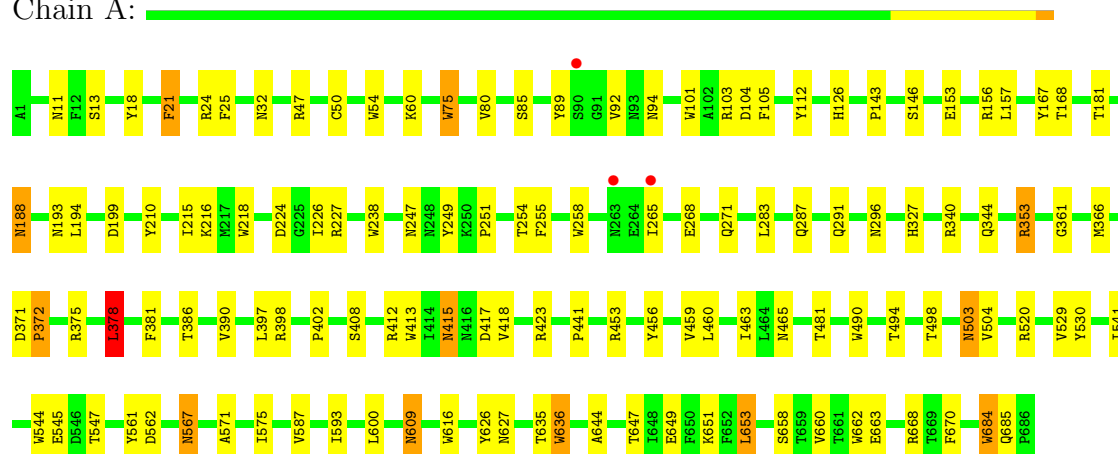
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	297	Total	O	0	0
			297	297		
3	B	307	Total	O	0	0
			307	307		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

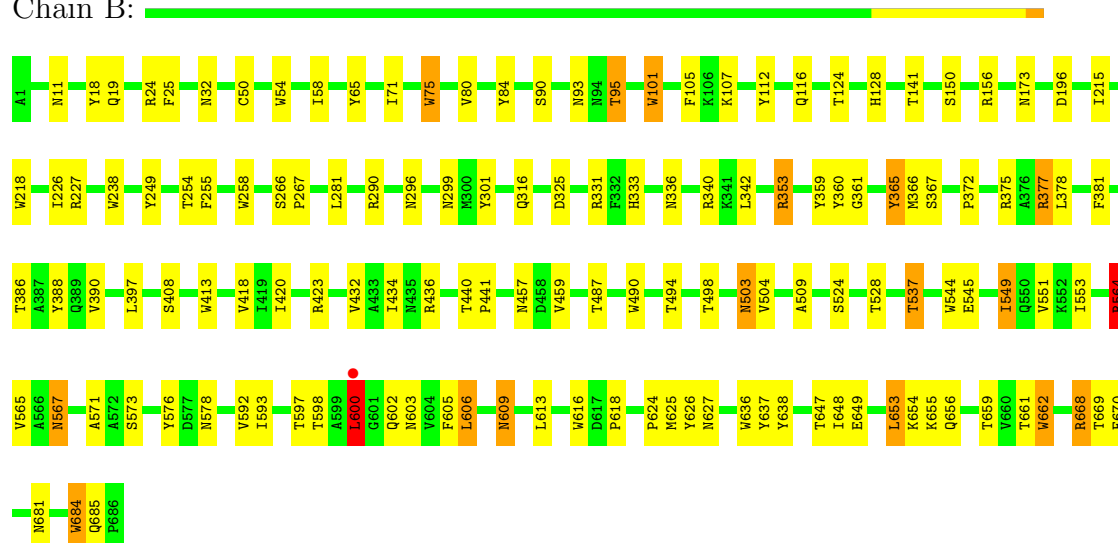
#### • Molecule 1: Cyclomaltodextrin glucanotransferase

Chain A:



#### • Molecule 1: Cyclomaltodextrin glucanotransferase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.93Å 73.66Å 78.20Å 85.11° 104.96° 100.97°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.2 (10.00-2.00) 86.2 (10.00-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.170 , 0.242 0.149 , 0.209	Depositor DCC
$R_{free}$ test set	4750 reflections (6.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78142 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.87	0/5442	1.48	63/7424 (0.8%)
1	B	0.86	1/5442 (0.0%)	1.49	70/7424 (0.9%)
All	All	0.87	1/10884 (0.0%)	1.49	133/14848 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	TRP	CG-CD2	-6.20	1.33	1.43

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	A	398	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	B	564	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	B	490	TRP	CD1-CG-CD2	9.22	113.67	106.30
1	A	616	TRP	CD1-CG-CD2	9.05	113.54	106.30
1	B	75	TRP	CD1-CG-CD2	9.01	113.51	106.30
1	A	75	TRP	CD1-CG-CD2	8.94	113.45	106.30
1	B	564	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	112	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	A	24	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	101	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	561	TYR	CB-CG-CD2	-8.47	115.92	121.00
1	A	544	TRP	CD1-CG-CD2	8.39	113.02	106.30
1	B	684	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	684	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	A	662	TRP	CD1-CG-CD2	8.28	112.93	106.30
1	A	636	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	B	662	TRP	CD1-CG-CD2	8.15	112.82	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	B	490	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	A	218	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	A	616	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	B	218	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	B	616	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	684	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	B	95	THR	N-CA-CB	-7.92	95.24	110.30
1	B	101	TRP	CD1-CG-CD2	7.92	112.63	106.30
1	A	75	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	A	353	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	B	413	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	B	636	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	B	662	TRP	CE2-CD2-CG	-7.77	101.09	107.30
1	B	637	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	B	290	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	B	684	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	544	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	B	238	TRP	CD1-CG-CD2	7.58	112.37	106.30
1	B	413	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	B	616	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	B	544	TRP	CD1-CG-CD2	7.52	112.31	106.30
1	A	218	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	636	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	A	54	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	B	340	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	112	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	A	375	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	490	TRP	CD1-CG-CD2	7.31	112.14	106.30
1	A	662	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	B	75	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	413	TRP	CD1-CG-CD2	7.27	112.12	106.30
1	A	24	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	54	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	B	375	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	388	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	A	413	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	B	218	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	B	636	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B	238	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	B	249	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	B	377	ARG	NE-CZ-NH1	-6.95	116.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	B	258	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	A	258	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	B	544	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	A	258	TRP	CD1-CG-CD2	6.80	111.74	106.30
1	B	24	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	412	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	249	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	A	47	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	101	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	B	662	TRP	CG-CD2-CE3	6.45	139.71	133.90
1	A	378	LEU	CB-CG-CD2	-6.41	100.11	111.00
1	A	490	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	B	75	TRP	CG-CD1-NE1	-6.26	103.84	110.10
1	A	398	ARG	CG-CD-NE	-6.22	98.75	111.80
1	B	325	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	375	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	75	TRP	CG-CD1-NE1	-6.14	103.96	110.10
1	B	365	TYR	CB-CG-CD2	-6.09	117.34	121.00
1	B	24	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	18	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	B	413	TRP	CB-CG-CD1	-6.03	119.16	127.00
1	A	238	TRP	CE2-CD2-CG	-6.02	102.49	107.30
1	B	54	TRP	CE2-CD2-CG	-6.00	102.50	107.30
1	A	75	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	A	50	CYS	CA-CB-SG	-5.98	103.24	114.00
1	B	258	TRP	CE2-CD2-CG	-5.97	102.53	107.30
1	B	626	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	B	54	TRP	CD1-CG-CD2	5.91	111.03	106.30
1	B	84	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	B	238	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	B	436	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	662	TRP	CB-CG-CD1	-5.79	119.47	127.00
1	B	413	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	B	684	TRP	CG-CD2-CE3	5.74	139.06	133.90
1	A	167	TYR	CB-CG-CD1	-5.66	117.61	121.00
1	A	238	TRP	CD1-CG-CD2	5.65	110.82	106.30
1	B	457	ASN	CB-CA-C	-5.57	99.27	110.40
1	B	301	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	B	545	GLU	CA-CB-CG	5.51	125.53	113.40
1	A	413	TRP	CB-CG-CD1	-5.50	119.85	127.00
1	A	103	ARG	NE-CZ-NH1	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	LEU	CA-CB-CG	5.46	127.87	115.30
1	B	156	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	196	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	616	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	A	456	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	B	218	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	B	353	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	377	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	B	490	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	375	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	616	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	A	541	ILE	N-CA-C	-5.30	96.68	111.00
1	B	18	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	B	359	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	101	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	216	LYS	CB-CG-CD	-5.26	97.92	111.60
1	B	606	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	544	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	A	530	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	B	684	TRP	CB-CG-CD1	-5.21	120.23	127.00
1	A	101	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	B	331	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	258	TRP	N-CA-C	-5.17	97.05	111.00
1	A	684	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	B	65	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	684	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	662	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	112	TYR	CB-CG-CD1	5.03	124.02	121.00
1	A	104	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	545	GLU	CA-CB-CG	5.03	124.46	113.40
1	B	576	TYR	CB-CG-CD1	-5.03	117.98	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5309	0	5051	52	0
1	B	5309	0	5051	56	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	297	0	0	3	0
3	B	307	0	0	6	0
All	All	11226	0	10102	108	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:340:ARG:HH12	1:A:465:ASN:HD22	1.35	0.73
1:B:564:ARG:HD2	1:B:573:SER:O	1.95	0.66
1:B:124:THR:O	1:B:128:HIS:HD2	1.83	0.61
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.83	0.61
1:A:651:LYS:HE2	1:A:663:GLU:O	2.00	0.61
1:A:361:GLY:HA3	1:A:366:MET:SD	2.42	0.59
1:B:80:VAL:HB	1:B:105:PHE:HA	1.86	0.57
1:B:361:GLY:HA3	1:B:366:MET:SD	2.45	0.56
1:A:11:ASN:ND2	3:A:1166:HOH:O	2.38	0.56
1:A:609:ASN:ND2	1:A:649:GLU:H	2.05	0.55
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.88	0.55
1:B:333:HIS:HD2	3:B:758:HOH:O	1.89	0.55
1:B:397:LEU:HD11	1:B:459:VAL:HG11	1.87	0.55
1:B:316:GLN:HG2	3:B:1262:HOH:O	2.07	0.55
1:B:600:LEU:HG	1:B:656:GLN:NE2	2.21	0.55
1:A:126:HIS:HE1	1:A:224:ASP:OD2	1.90	0.55
1:A:397:LEU:HD11	1:A:459:VAL:HG11	1.87	0.55
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.43	0.54
1:B:11:ASN:ND2	3:B:1259:HOH:O	2.40	0.54
1:B:605:PHE:HB2	1:B:653:LEU:HG	1.90	0.54
1:A:567:ASN:ND2	1:A:571:ALA:H	2.05	0.54
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.43	0.53
1:B:434:ILE:HG12	1:B:487:THR:HG23	1.90	0.53
1:B:528:THR:HG23	1:B:537:THR:HG23	1.90	0.53
1:B:653:LEU:HD12	1:B:655:LYS:HG3	1.91	0.52
1:B:316:GLN:HE22	1:B:578:ASN:HD22	1.56	0.52
1:B:605:PHE:CE1	1:B:655:LYS:HB2	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:415:ASN:ND2	1:A:417:ASP:H	2.07	0.52
1:A:247:ASN:HA	1:A:251:PRO:HB3	1.92	0.52
1:B:226:ILE:HB	1:B:254:THR:HG23	1.92	0.51
1:A:25:PHE:HB3	3:A:1175:HOH:O	2.09	0.51
1:A:80:VAL:HB	1:A:105:PHE:HA	1.93	0.50
1:A:441:PRO:HB2	1:A:481:THR:CG2	2.42	0.50
1:B:75:TRP:CZ2	1:B:227:ARG:HG3	2.47	0.50
1:A:653:LEU:HD12	1:A:660:VAL:HG13	1.94	0.49
1:A:520:ARG:HD3	1:A:547:THR:HG22	1.94	0.49
1:A:193:ASN:OD1	1:A:199:ASP:HB2	2.12	0.49
1:B:408:SER:O	1:B:423:ARG:HA	2.13	0.49
1:B:598:THR:HG22	1:B:654:LYS:HD2	1.95	0.48
1:A:92:VAL:HG13	1:A:94:ASN:HD21	1.79	0.48
1:B:649:GLU:HA	1:B:668:ARG:O	2.14	0.48
1:B:93:ASN:HB2	3:B:977:HOH:O	2.14	0.48
1:A:567:ASN:HD21	1:A:571:ALA:H	1.61	0.47
1:A:21:PHE:HE2	1:A:327:HIS:HB3	1.80	0.47
1:B:25:PHE:HB3	3:B:717:HOH:O	2.14	0.47
1:A:153:GLU:O	1:A:156:ARG:HG3	2.15	0.47
1:A:146:SER:HA	1:A:168:THR:OG1	2.14	0.47
1:A:587:VAL:HG13	1:A:644:ALA:HB2	1.97	0.47
1:A:668:ARG:NH1	1:A:685:GLN:HG3	2.30	0.46
1:A:415:ASN:HD22	1:A:418:VAL:H	1.63	0.46
1:B:342:LEU:HD23	1:B:365:TYR:CD1	2.50	0.46
1:B:50:CYS:HB3	1:B:377:ARG:HH11	1.79	0.46
1:B:71:ILE:HD13	1:B:71:ILE:HA	1.72	0.46
1:A:340:ARG:O	1:A:344:GLN:HG3	2.15	0.46
1:B:418:VAL:HA	1:B:434:ILE:O	2.15	0.46
1:A:89:TYR:O	1:A:92:VAL:HG12	2.15	0.46
1:B:603:ASN:HB3	1:B:624:PRO:HB3	1.98	0.46
1:A:386:THR:O	1:A:390:VAL:HG23	2.16	0.46
1:B:593:ILE:HD13	1:B:684:TRP:HE3	1.82	0.45
1:B:564:ARG:HG3	1:B:565:VAL:N	2.32	0.45
1:B:386:THR:O	1:B:390:VAL:HG23	2.17	0.45
1:B:618:PRO:HG3	1:B:662:TRP:CZ2	2.52	0.44
1:A:503:ASN:HD22	1:A:504:VAL:H	1.66	0.44
1:B:58:ILE:HG23	1:B:124:THR:HG21	2.00	0.44
1:A:460:LEU:O	1:A:463:ILE:HG12	2.18	0.44
1:B:549:ILE:HD11	1:B:551:VAL:HB	1.99	0.44
1:B:266:SER:HA	1:B:267:PRO:HD3	1.84	0.44
1:A:647:THR:HA	1:A:670:PHE:O	2.18	0.44
1:B:420:ILE:HA	1:B:432:VAL:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:371:ASP:HA	1:A:372:PRO:HA	1.78	0.44
1:A:21:PHE:CE2	1:A:327:HIS:HB3	2.54	0.43
1:B:648:ILE:O	1:B:669:THR:HA	2.18	0.43
1:B:609:ASN:ND2	1:B:649:GLU:H	2.16	0.43
1:B:592:VAL:HB	1:B:681:ASN:HA	1.99	0.43
1:B:378:LEU:HD21	1:B:381:PHE:CZ	2.53	0.43
1:A:296:ASN:HB2	3:A:774:HOH:O	2.17	0.43
1:B:647:THR:HA	1:B:670:PHE:O	2.18	0.43
1:A:593:ILE:O	1:A:635:THR:HA	2.19	0.43
1:A:283:LEU:O	1:A:287:GLN:HG2	2.19	0.43
1:A:227:ARG:HG2	1:A:255:PHE:CE1	2.54	0.43
1:A:408:SER:O	1:A:423:ARG:HA	2.19	0.43
1:B:567:ASN:ND2	1:B:571:ALA:H	2.17	0.43
1:B:598:THR:HB	1:B:602:GLN:HB3	2.00	0.42
1:B:603:ASN:O	1:B:654:LYS:HA	2.19	0.42
1:B:503:ASN:HD22	1:B:504:VAL:H	1.67	0.42
1:A:181:THR:HA	1:A:188:ASN:HD21	1.84	0.42
1:B:101:TRP:HA	1:B:141:THR:O	2.20	0.42
1:A:626:TYR:O	1:A:636:TRP:HA	2.19	0.42
1:A:287:GLN:O	1:A:291:GLN:HG3	2.20	0.42
1:A:378:LEU:HD21	1:A:381:PHE:CE1	2.54	0.42
1:B:227:ARG:HA	1:B:255:PHE:O	2.20	0.42
1:B:19:GLN:O	1:B:360:TYR:HB3	2.20	0.42
1:B:440:THR:HA	1:B:441:PRO:HD3	1.92	0.41
1:A:402:PRO:HG3	1:A:520:ARG:CZ	2.51	0.41
1:B:50:CYS:HB3	1:B:377:ARG:NH1	2.35	0.41
1:B:509:ALA:HB3	1:B:553:ILE:CD1	2.51	0.41
1:A:215:ILE:HA	1:A:215:ILE:HD12	1.91	0.41
1:A:340:ARG:HH12	1:A:465:ASN:ND2	2.10	0.41
1:B:656:GLN:O	1:B:659:THR:HG22	2.20	0.41
1:B:215:ILE:HA	1:B:215:ILE:HD12	1.91	0.41
1:B:624:PRO:HD2	3:B:1276:HOH:O	2.20	0.41
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.78	0.41
1:A:649:GLU:HA	1:A:668:ARG:O	2.21	0.40
1:A:157:LEU:HD11	1:A:210:TYR:CE2	2.56	0.40
1:A:226:ILE:O	1:A:254:THR:HA	2.22	0.40
1:A:593:ILE:HD11	1:A:684:TRP:HA	2.03	0.40
1:B:80:VAL:HA	1:B:107:LYS:O	2.21	0.40
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	684/686 (100%)	667 (98%)	17 (2%)	0	100	100
1	B	684/686 (100%)	661 (97%)	21 (3%)	2 (0%)	50	44
All	All	1368/1372 (100%)	1328 (97%)	38 (3%)	2 (0%)	59	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	SER
1	B	600	LEU

### 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	564/564 (100%)	540 (96%)	24 (4%)	40	33
1	B	564/564 (100%)	535 (95%)	29 (5%)	33	26
All	All	1128/1128 (100%)	1075 (95%)	53 (5%)	36	29

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	21	PHE
1	A	32	ASN
1	A	85	SER
1	A	143	PRO
1	A	188	ASN
1	A	265	ILE

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Mol	Chain	Res	Type
1	A	268	GLU
1	A	271	GLN
1	A	353	ARG
1	A	372	PRO
1	A	378	LEU
1	A	415	ASN
1	A	453	ARG
1	A	494	THR
1	A	498	THR
1	A	503	ASN
1	A	529	VAL
1	A	567	ASN
1	A	600	LEU
1	A	609	ASN
1	A	627	ASN
1	A	653	LEU
1	A	658	SER
1	B	32	ASN
1	B	95	THR
1	B	116	GLN
1	B	150	SER
1	B	173	ASN
1	B	296	ASN
1	B	299	ASN
1	B	336	ASN
1	B	353	ARG
1	B	367	SER
1	B	372	PRO
1	B	494	THR
1	B	498	THR
1	B	503	ASN
1	B	524	SER
1	B	537	THR
1	B	549	ILE
1	B	564	ARG
1	B	567	ASN
1	B	597	THR
1	B	600	LEU
1	B	606	LEU
1	B	609	ASN
1	B	613	LEU
1	B	627	ASN

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Mol	Chain	Res	Type
1	B	653	LEU
1	B	661	THR
1	B	668	ARG
1	B	685	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	32	ASN
1	A	55	GLN
1	A	59	ASN
1	A	94	ASN
1	A	126	HIS
1	A	128	HIS
1	A	188	ASN
1	A	415	ASN
1	A	465	ASN
1	A	503	ASN
1	A	567	ASN
1	A	578	ASN
1	A	609	ASN
1	A	627	ASN
1	B	11	ASN
1	B	32	ASN
1	B	33	ASN
1	B	188	ASN
1	B	271	GLN
1	B	299	ASN
1	B	316	GLN
1	B	333	HIS
1	B	465	ASN
1	B	503	ASN
1	B	548	GLN
1	B	567	ASN
1	B	609	ASN
1	B	627	ASN
1	B	656	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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	686/686 (100%)	-0.82	3 (0%) 90 91	9, 17, 31, 71	0
1	B	686/686 (100%)	-0.71	1 (0%) 93 94	11, 20, 39, 60	0
All	All	1372/1372 (100%)	-0.77	4 (0%) 91 93	9, 18, 37, 71	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	SER	2.8
1	B	600	LEU	2.5
1	A	265	ILE	2.1
1	A	263	ASN	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	689	1/1	0.06	-1.30	18,18,18,18	0
2	CA	A	688	1/1	0.05	-1.88	19,19,19,19	0
2	CA	A	687	1/1	0.04	-2.57	13,13,13,13	0
2	CA	B	690	1/1	0.04	-3.89	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.