Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 01:08 AM EDT

PDB ID	:	1V3K
Title	:	Crystal structure of F283Y 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 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 (i) 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 (1)) were used in the production of this report:

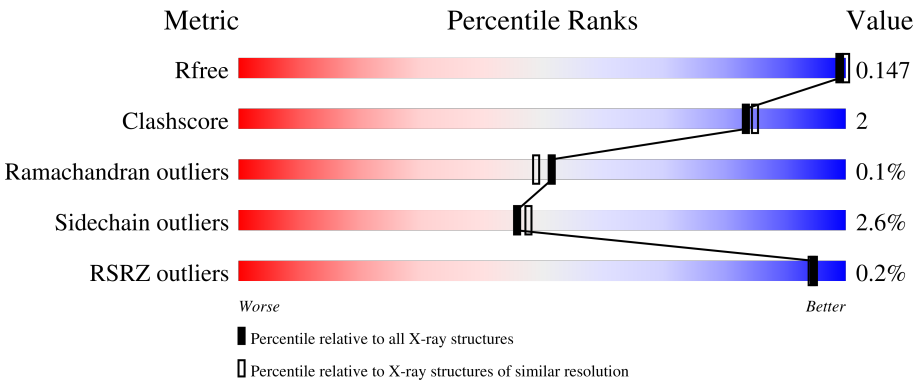
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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 <=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	686	90% 9% •
1	B	686	88% 11% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11435 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 Cyclomaltodextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	686	5313	3354	906	1037	16	0	0	0
1	B	686	5313	3354	906	1037	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	TYR	PHE	engineered mutation	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	283	TYR	PHE	engineered mutation	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
			Total	Ca		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

- Molecule 3 is water.

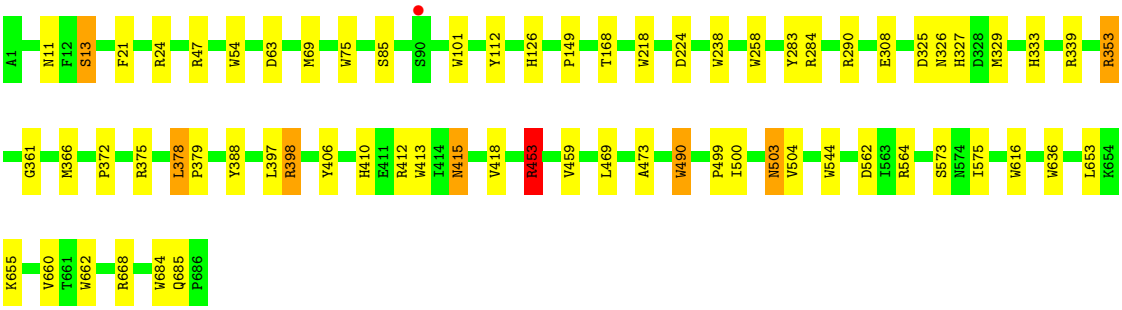
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	436	436	436	0	0
3	B	369	369	369	0	0

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 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.

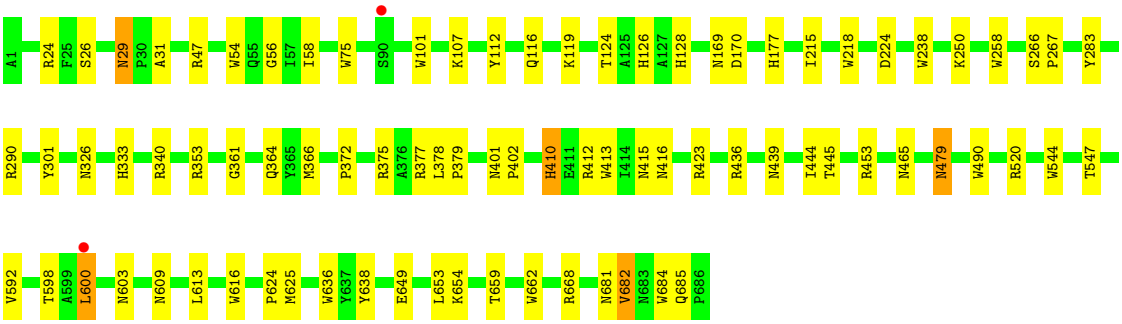
• Molecule 1: Cyclomaltodextrin glucanotransferase

Chain A:



• Molecule 1: Cyclomaltodextrin glucanotransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.88Å 74.43Å 79.01Å 85.15° 105.05° 101.02°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.1 (10.00-2.00) 90.1 (10.00-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.90 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.155 , 0.200 0.148 , 0.147	Depositor DCC
R_{free} test set	5099 reflections (6.03%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11435	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.74	0/5447	1.37	62/7431 (0.8%)
1	B	0.75	0/5447	1.33	52/7431 (0.7%)
All	All	0.75	0/10894	1.35	114/14862 (0.8%)

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398	ARG	NE-CZ-NH2	-24.55	108.02	120.30
1	A	398	ARG	NE-CZ-NH1	14.11	127.35	120.30
1	B	413	TRP	CD1-CG-CD2	9.09	113.57	106.30
1	A	353	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	54	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	616	TRP	CD1-CG-CD2	8.58	113.16	106.30
1	B	662	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	636	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	112	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	A	662	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	A	413	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	398	ARG	CG-CD-NE	-8.16	94.67	111.80
1	A	54	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	A	490	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	A	101	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	B	238	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	A	616	TRP	CE2-CD2-CG	-7.82	101.04	107.30
1	B	616	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	B	24	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	413	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	218	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	B	662	TRP	CE2-CD2-CG	-7.67	101.16	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	636	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	A	684	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	B	436	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	B	490	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	B	101	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	B	684	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	B	636	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	B	684	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	47	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	B	75	TRP	CD1-CG-CD2	7.43	112.25	106.30
1	A	238	TRP	CD1-CG-CD2	7.41	112.22	106.30
1	A	75	TRP	CD1-CG-CD2	7.37	112.19	106.30
1	A	218	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	B	636	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	B	616	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	B	283	TYR	CB-CG-CD1	-7.19	116.68	121.00
1	B	101	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	258	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	B	218	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	A	413	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	A	101	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	544	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	B	544	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	B	238	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	544	TRP	CD1-CG-CD2	6.84	111.77	106.30
1	A	75	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	B	436	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	662	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	B	490	TRP	CE2-CD2-CG	-6.81	101.86	107.30
1	A	684	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	B	544	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	B	75	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	B	54	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	A	238	TRP	CE2-CD2-CG	-6.63	101.99	107.30
1	B	290	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	B	54	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	616	TRP	CG-CD2-CE3	6.56	139.80	133.90
1	B	218	TRP	CE2-CD2-CG	-6.47	102.13	107.30
1	B	258	TRP	CD1-CG-CD2	6.42	111.43	106.30
1	B	112	TYR	CB-CG-CD2	-6.39	117.16	121.00
1	A	258	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	A	375	ARG	NE-CZ-NH2	-6.37	117.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	490	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	A	353	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	453	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	75	TRP	CG-CD2-CE3	6.13	139.41	133.90
1	A	290	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	B	47	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	258	TRP	CE2-CD2-CG	-6.06	102.45	107.30
1	B	412	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	413	TRP	CG-CD1-NE1	-5.95	104.15	110.10
1	A	24	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	218	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	A	453	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	682	VAL	N-CA-CB	-5.87	98.60	111.50
1	A	412	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	238	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	B	684	TRP	CG-CD2-CE3	5.78	139.10	133.90
1	B	301	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	564	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	A	47	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	616	TRP	CG-CD2-CE3	5.62	138.95	133.90
1	A	616	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	A	375	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	413	TRP	CB-CG-CD1	-5.58	119.75	127.00
1	A	238	TRP	CB-CG-CD1	-5.53	119.81	127.00
1	B	662	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	B	616	TRP	CB-CG-CD1	-5.52	119.83	127.00
1	A	339	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	238	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	412	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	339	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	75	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	A	406	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	A	283	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	B	444	ILE	CA-C-N	-5.30	105.55	117.20
1	B	662	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	B	423	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	413	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	54	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	B	375	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	413	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	B	453	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	284	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	636	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	B	107	LYS	CB-CG-CD	-5.14	98.25	111.60
1	A	616	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	A	54	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	A	636	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	A	662	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	63	ASP	CB-CG-OD1	5.02	122.81	118.30

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	5313	0	5050	26	0
1	B	5313	0	5050	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	436	0	0	4	0
3	B	369	0	0	1	0
All	All	11435	0	10100	50	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 2.

All (50) 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:325:ASP:HA	1:A:329:MET:HE2	1.61	0.81
1:B:378:LEU:HD12	1:B:379:PRO:HD2	1.70	0.72
1:A:325:ASP:HA	1:A:329:MET:CE	2.26	0.65
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.82	0.61
1:A:11:ASN:ND2	3:A:1743:HOH:O	2.36	0.58
1:B:361:GLY:HA3	1:B:366:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HH12	1:B:465:ASN:ND2	2.02	0.57
1:B:592:VAL:HB	1:B:681:ASN:HA	1.88	0.56
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.89	0.56
1:A:378:LEU:HD23	1:A:379:PRO:HD2	1.87	0.55
1:A:503:ASN:HD22	1:A:504:VAL:H	1.55	0.55
1:A:149:PRO:HG3	1:A:168:THR:HG21	1.89	0.54
1:A:453:ARG:HH22	1:A:473:ALA:HB2	1.73	0.54
1:A:126:HIS:HE1	1:A:224:ASP:OD2	1.93	0.52
1:A:653:LEU:HD12	1:A:660:VAL:HG13	1.90	0.52
1:B:124:THR:O	1:B:128:HIS:HD2	1.92	0.51
1:B:340:ARG:HH12	1:B:465:ASN:HD22	1.58	0.51
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.93	0.50
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.94	0.50
1:A:21:PHE:HE2	1:A:327:HIS:HB3	1.77	0.49
1:A:453:ARG:HH12	1:A:473:ALA:HA	1.78	0.49
1:B:29:ASN:HD21	1:B:31:ALA:HB3	1.77	0.49
1:A:333:HIS:HD2	3:A:1769:HOH:O	1.95	0.49
1:B:598:THR:HG22	1:B:654:LYS:HD2	1.95	0.49
1:A:655:LYS:HG2	1:A:660:VAL:HG22	1.94	0.48
1:B:58:ILE:HG23	1:B:124:THR:HG21	1.97	0.47
1:B:603:ASN:HB3	1:B:624:PRO:HB3	1.98	0.45
1:A:126:HIS:HD2	3:A:1755:HOH:O	1.99	0.45
1:A:13:SER:O	1:A:398:ARG:HD3	2.17	0.44
1:B:333:HIS:HD2	3:B:1795:HOH:O	2.00	0.43
1:A:410:HIS:HB2	3:A:1392:HOH:O	2.18	0.43
1:B:625:MET:HG2	1:B:638:TYR:HB2	2.01	0.43
1:B:361:GLY:HA2	1:B:378:LEU:HD13	2.01	0.42
1:A:361:GLY:HA3	1:A:366:MET:SD	2.59	0.42
1:B:445:THR:HG22	1:B:479:ASN:OD1	2.18	0.42
1:B:364:GLN:HG3	1:B:378:LEU:HD11	2.00	0.42
1:B:26:SER:O	1:B:56:GLY:HA3	2.19	0.42
1:B:215:ILE:HD12	1:B:215:ILE:HA	1.89	0.42
1:B:401:ASN:HA	1:B:402:PRO:HD2	1.91	0.42
1:B:520:ARG:HD3	1:B:547:THR:HG22	2.01	0.42
1:B:266:SER:HA	1:B:267:PRO:HD2	1.90	0.41
1:A:308:GLU:OE2	1:B:410:HIS:HE1	2.04	0.41
1:A:397:LEU:HD11	1:A:459:VAL:HG11	2.03	0.41
1:B:668:ARG:NH1	1:B:685:GLN:HG3	2.35	0.41
1:A:69:MET:HG3	1:A:388:TYR:CE1	2.56	0.41
1:A:503:ASN:HD22	1:A:504:VAL:N	2.19	0.41
1:A:415:ASN:HD22	1:A:418:VAL:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HB2	1:A:490:TRP:CE2	2.56	0.41
1:B:649:GLU:HA	1:B:668:ARG:O	2.22	0.40
1:A:668:ARG:NH1	1:A:685:GLN:HG3	2.36	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	684/686 (100%)	669 (98%)	15 (2%)	0	100	100
1	B	684/686 (100%)	668 (98%)	15 (2%)	1 (0%)	51	49
All	All	1368/1372 (100%)	1337 (98%)	30 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	LEU

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	564/564 (100%)	554 (98%)	10 (2%)	59	63
1	B	564/564 (100%)	545 (97%)	19 (3%)	37	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1128/1128 (100%)	1099 (97%)	29 (3%)	46 48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	85	SER
1	A	326	ASN
1	A	353	ARG
1	A	372	PRO
1	A	378	LEU
1	A	415	ASN
1	A	453	ARG
1	A	500	ILE
1	A	503	ASN
1	B	29	ASN
1	B	116	GLN
1	B	119	LYS
1	B	169	ASN
1	B	250	LYS
1	B	326	ASN
1	B	353	ARG
1	B	372	PRO
1	B	410	HIS
1	B	415	ASN
1	B	416	ASN
1	B	439	ASN
1	B	479	ASN
1	B	600	LEU
1	B	609	ASN
1	B	613	LEU
1	B	653	LEU
1	B	659	THR
1	B	682	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	55	GLN
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	62	ASN
1	A	116	GLN
1	A	120	ASN
1	A	126	HIS
1	A	296	ASN
1	A	326	ASN
1	A	333	HIS
1	A	415	ASN
1	A	503	ASN
1	A	656	GLN
1	B	29	ASN
1	B	62	ASN
1	B	88	ASN
1	B	93	ASN
1	B	126	HIS
1	B	128	HIS
1	B	177	HIS
1	B	326	ASN
1	B	333	HIS
1	B	410	HIS
1	B	415	ASN
1	B	465	ASN
1	B	548	GLN
1	B	609	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	686/686 (100%)	-0.92	1 (0%)	95	95	4, 11, 24, 42	0
1	B	686/686 (100%)	-0.76	2 (0%)	94	93	5, 15, 33, 49	0
All	All	1372/1372 (100%)	-0.84	3 (0%)	95	94	4, 13, 29, 49	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	3.5
1	A	90	SER	3.1
1	B	90	SER	2.5

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(Å^2)	Q<0.9
2	CA	A	687	1/1	0.98	0.04	7,7,7,7	0
2	CA	B	689	1/1	0.99	0.04	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	B	690	1/1	0.99	0.02	13,13,13,13	0
2	CA	A	688	1/1	1.00	0.05	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.