Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 10:49 AM EDT

PDB ID	:	1CYG
Title	:	CYCLODEXTRIN GLUCANOTRANSFERASE (E.C.2.4.1.19) (CGTASE)
Authors	:	Kubota, M.; Matsuura, Y.; Sakai, S.; Katsube, Y.
Deposited on	:	1993-02-03
Resolution	:	2.50 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:

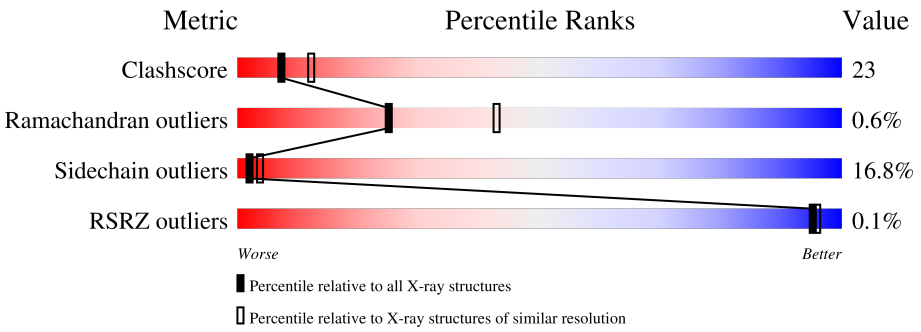
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	680	51% 38% 9% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5551 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 CYCLODEXTRIN GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	680	5318	3347	905	1044	22	0	0	0

- 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

- Molecule 3 is water.

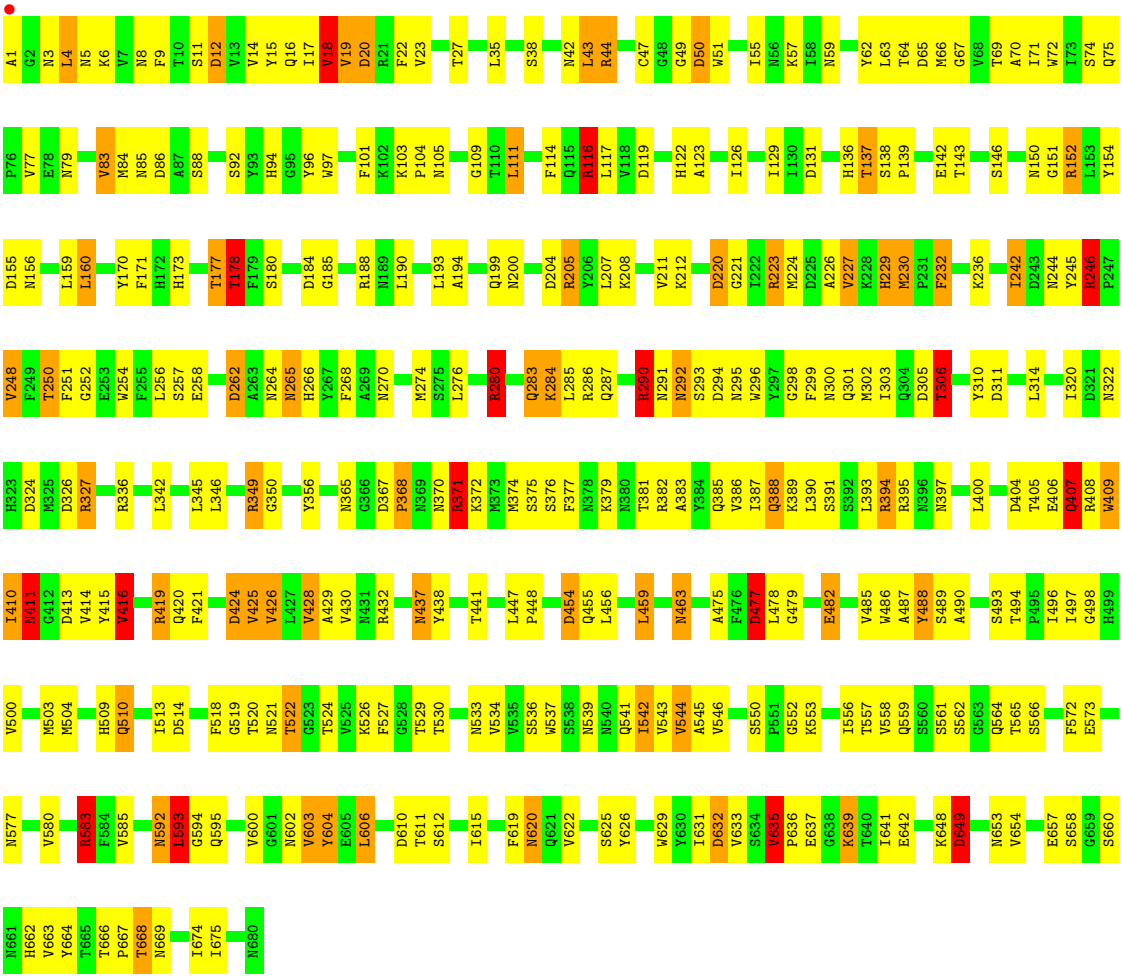
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	231	231	231	0	0

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: CYCLODEXTRIN GLUCANOTRANSFERASE

Chain A: 51% 38% 9%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.50Å 88.00Å 78.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.50 88.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.50) 52.9 (88.00-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.02Å)	Xtriage
Refinement program	PROFFT, PROLSQ	Depositor
R, R_{free}	0.154 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	9.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5551	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	0.96	0/5447	1.71	86/7411 (1.2%)

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	419	ARG	CD-NE-CZ	21.45	153.63	123.60
1	A	327	ARG	NE-CZ-NH1	15.39	128.00	120.30
1	A	246	ARG	NE-CZ-NH1	14.30	127.45	120.30
1	A	371	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	A	280	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	246	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	A	152	ARG	NE-CZ-NH1	11.73	126.17	120.30
1	A	152	ARG	CD-NE-CZ	10.95	138.93	123.60
1	A	394	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	A	152	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	A	395	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	395	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	583	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	327	ARG	CD-NE-CZ	9.16	136.43	123.60
1	A	205	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	583	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	290	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	583	ARG	CD-NE-CZ	8.83	135.97	123.60
1	A	280	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	A	324	ASP	CB-CG-OD1	-8.22	110.90	118.30
1	A	432	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	311	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	A	416	VAL	CB-CA-C	7.56	125.77	111.40
1	A	50	ASP	CB-CG-OD2	-7.44	111.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	394	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	44	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	649	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	408	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	488	TYR	CB-CG-CD1	-6.86	116.88	121.00
1	A	388	GLN	CA-CB-CG	6.86	128.49	113.40
1	A	246	ARG	CD-NE-CZ	6.84	133.17	123.60
1	A	477	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	382	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	424	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	306	THR	CA-CB-CG2	6.55	121.57	112.40
1	A	4	LEU	CB-CA-C	6.48	122.51	110.20
1	A	454	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	410	ILE	C-N-CA	6.43	137.77	121.70
1	A	390	LEU	CB-CA-C	6.34	122.25	110.20
1	A	290	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	336	ARG	CD-NE-CZ	6.25	132.35	123.60
1	A	230	MET	CB-CA-C	6.21	122.81	110.40
1	A	229	HIS	CA-CB-CG	-6.17	103.10	113.60
1	A	190	LEU	CB-CA-C	6.12	121.84	110.20
1	A	432	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	603	VAL	CB-CA-C	5.97	122.75	111.40
1	A	371	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	12	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	286	ARG	CD-NE-CZ	5.92	131.89	123.60
1	A	20	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	276	LEU	N-CA-CB	-5.87	98.67	110.40
1	A	262	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	160	LEU	CB-CA-C	5.82	121.26	110.20
1	A	178	THR	N-CA-CB	-5.78	99.31	110.30
1	A	577	ASN	N-CA-CB	-5.72	100.31	110.60
1	A	407	GLN	CA-CB-CG	5.71	125.97	113.40
1	A	65	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	116	ARG	CD-NE-CZ	-5.69	115.63	123.60
1	A	86	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	A	232	PHE	N-CA-CB	5.68	120.83	110.60
1	A	20	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	A	604	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	280	ARG	O-C-N	5.61	131.68	122.70
1	A	327	ARG	CA-CB-CG	5.57	125.65	113.40
1	A	18	VAL	CB-CA-C	5.52	121.89	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	632	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	635	VAL	N-CA-CB	-5.36	99.70	111.50
1	A	154	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	336	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	327	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	A	136	HIS	CA-CB-CG	-5.28	104.63	113.60
1	A	305	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	367	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	211	VAL	CB-CA-C	5.26	121.39	111.40
1	A	205	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	223	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	119	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	220	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	205	ARG	CD-NE-CZ	5.21	130.89	123.60
1	A	286	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	521	ASN	CB-CA-C	5.14	120.67	110.40
1	A	411	ASN	CB-CA-C	-5.12	100.16	110.40
1	A	155	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	463	ASN	N-CA-CB	-5.03	101.55	110.60
1	A	383	ALA	CB-CA-C	5.02	117.63	110.10

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	5318	0	5029	233	0
2	A	2	0	0	0	0
3	A	231	0	0	14	0
All	All	5551	0	5029	233	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 23.

All (233) 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:592:ASN:HB3	1:A:593:LEU:HD23	1.40	1.03
1:A:137:THR:HG22	1:A:194:ALA:HB3	1.45	0.99
1:A:177:THR:HG22	1:A:188:ARG:HB2	1.44	0.99
1:A:557:THR:HG21	1:A:565:THR:HG23	1.44	0.98
1:A:519:GLY:H	1:A:539:ASN:ND2	1.67	0.93
1:A:519:GLY:N	1:A:539:ASN:HD22	1.66	0.91
1:A:306:THR:CG2	1:A:349:ARG:HH21	1.83	0.91
1:A:306:THR:HG21	1:A:349:ARG:HH21	1.35	0.91
1:A:409:TRP:HB3	1:A:416:VAL:HG13	1.54	0.89
1:A:519:GLY:H	1:A:539:ASN:HD22	0.88	0.88
1:A:258:GLU:HG3	1:A:287:GLN:NE2	1.91	0.86
1:A:79:ASN:HD22	1:A:92:SER:HB2	1.44	0.82
1:A:244:ASN:HD22	1:A:509:HIS:HE1	1.27	0.82
1:A:290:ARG:HH11	1:A:291:ASN:HD21	1.28	0.81
1:A:258:GLU:HG3	1:A:287:GLN:HE21	1.48	0.79
1:A:244:ASN:HD22	1:A:509:HIS:CE1	2.01	0.79
1:A:137:THR:CG2	1:A:194:ALA:HB3	2.13	0.78
1:A:15:TYR:HB3	1:A:71:ILE:HD12	1.66	0.77
1:A:503:MET:HA	1:A:503:MET:HE2	1.66	0.76
1:A:137:THR:HG23	1:A:138:SER:H	1.50	0.76
1:A:557:THR:CG2	1:A:565:THR:HG23	2.15	0.76
1:A:280:ARG:HD2	3:A:863:HOH:O	1.85	0.75
1:A:583:ARG:HD3	1:A:632:ASP:OD1	1.85	0.75
1:A:66:MET:HE2	1:A:387:ILE:HD13	1.67	0.74
1:A:177:THR:HG21	1:A:185:GLY:HA2	1.69	0.74
1:A:64:THR:HG22	1:A:126:ILE:HD11	1.69	0.74
1:A:221:GLY:HA2	1:A:248:VAL:HG13	1.67	0.74
1:A:585:VAL:HB	1:A:675:ILE:HG12	1.69	0.73
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.52	0.73
1:A:419:ARG:HB2	1:A:426:VAL:HG13	1.69	0.73
1:A:185:GLY:O	3:A:912:HOH:O	2.06	0.72
1:A:246:ARG:HD3	1:A:246:ARG:C	2.10	0.72
1:A:437:ASN:ND2	1:A:438:TYR:N	2.37	0.72
1:A:385:GLN:HA	1:A:388:GLN:HE21	1.58	0.69
1:A:611:THR:HG21	1:A:654:VAL:HG11	1.74	0.69
1:A:510:GLN:HE21	1:A:510:GLN:HA	1.58	0.69
1:A:411:ASN:HB2	1:A:414:VAL:H	1.58	0.68
1:A:280:ARG:O	1:A:284:LYS:HB2	1.92	0.68
1:A:62:TYR:HA	1:A:379:LYS:HE2	1.75	0.68
1:A:122:HIS:HE1	1:A:220:ASP:OD2	1.76	0.68
1:A:266:HIS:CE1	1:A:280:ARG:HH21	2.13	0.67
1:A:592:ASN:HB3	1:A:593:LEU:CD2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:OD1	1:A:489:SER:HA	1.94	0.67
1:A:664:TYR:OH	1:A:667:PRO:HD3	1.96	0.66
1:A:177:THR:HG22	1:A:188:ARG:CB	2.25	0.66
1:A:635:VAL:HG22	1:A:636:PRO:HD2	1.76	0.66
1:A:298:GLY:O	1:A:301:GLN:HG2	1.96	0.65
1:A:411:ASN:HB3	1:A:413:ASP:H	1.60	0.65
1:A:137:THR:CG2	1:A:138:SER:H	2.10	0.65
1:A:534:VAL:HB	1:A:544:VAL:HG23	1.79	0.64
1:A:649:ASP:CG	1:A:653:ASN:HB2	2.19	0.63
1:A:104:PRO:HG3	1:A:111:LEU:HD13	1.80	0.63
1:A:224:MET:HG3	1:A:274:MET:CE	2.28	0.63
1:A:518:PHE:HB2	1:A:539:ASN:HA	1.81	0.63
1:A:227:VAL:HG12	1:A:254:TRP:HB2	1.80	0.62
1:A:416:VAL:HA	1:A:428:VAL:O	1.99	0.62
1:A:522:THR:HA	1:A:537:TRP:CG	2.34	0.62
1:A:557:THR:HG23	1:A:566:SER:O	2.00	0.62
1:A:109:GLY:HA2	3:A:803:HOH:O	1.99	0.62
1:A:649:ASP:HB2	1:A:653:ASN:HB2	1.81	0.62
1:A:35:LEU:HD13	1:A:83:VAL:HG22	1.82	0.61
1:A:79:ASN:ND2	1:A:97:TRP:H	1.98	0.61
1:A:494:THR:HG22	1:A:564:GLN:OE1	2.01	0.61
1:A:290:ARG:NH1	1:A:291:ASN:HD21	1.98	0.61
1:A:503:MET:HA	1:A:503:MET:CE	2.30	0.60
1:A:227:VAL:HG22	1:A:268:PHE:CZ	2.37	0.60
1:A:557:THR:HG22	1:A:558:VAL:N	2.16	0.60
1:A:226:ALA:HB1	1:A:229:HIS:CD2	2.38	0.59
1:A:400:LEU:CD2	1:A:426:VAL:HG11	2.31	0.59
1:A:404:ASP:O	1:A:419:ARG:HD2	2.01	0.59
1:A:79:ASN:HD21	1:A:97:TRP:H	1.49	0.59
1:A:244:ASN:ND2	1:A:509:HIS:HE1	1.98	0.59
1:A:292:ASN:ND2	3:A:729:HOH:O	2.22	0.59
1:A:77:VAL:CG2	1:A:101:PHE:HA	2.33	0.59
1:A:285:LEU:HD23	1:A:320:ILE:HG22	1.84	0.59
1:A:513:ILE:HD12	1:A:542:ILE:CD1	2.33	0.59
1:A:479:GLY:O	1:A:482:GLU:HB2	2.02	0.58
1:A:212:LYS:HE2	1:A:245:TYR:CD1	2.38	0.58
1:A:14:VAL:HG22	1:A:70:ALA:HB3	1.84	0.58
1:A:648:LYS:HA	1:A:653:ASN:O	2.03	0.58
1:A:150:ASN:HB3	1:A:152:ARG:HD3	1.85	0.57
1:A:370:ASN:OD1	1:A:371:ARG:HD2	2.04	0.57
1:A:509:HIS:O	1:A:545:ALA:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ASP:OD1	1:A:612:SER:HB2	2.04	0.57
1:A:559:GLN:HA	1:A:564:GLN:O	2.04	0.57
1:A:552:GLY:HA2	1:A:604:TYR:CE1	2.40	0.57
1:A:17:ILE:HD12	1:A:71:ILE:HG13	1.87	0.56
1:A:226:ALA:HB1	1:A:229:HIS:HD2	1.69	0.56
1:A:236:LYS:HD2	1:A:504:MET:HE1	1.86	0.56
1:A:503:MET:HE2	1:A:572:PHE:HD2	1.70	0.56
1:A:177:THR:HB	1:A:184:ASP:OD2	2.06	0.56
1:A:488:TYR:OH	1:A:490:ALA:HB2	2.04	0.56
1:A:557:THR:HG21	1:A:565:THR:CG2	2.26	0.56
1:A:350:GLY:O	1:A:394:ARG:NH2	2.39	0.56
1:A:77:VAL:HG21	1:A:101:PHE:HA	1.87	0.56
1:A:302:MET:O	1:A:306:THR:HB	2.07	0.55
1:A:637:GLU:HB2	1:A:668:THR:HA	1.89	0.55
1:A:44:ARG:HD2	1:A:88:SER:CB	2.37	0.55
1:A:389:LYS:HE3	1:A:459:LEU:HD22	1.89	0.55
1:A:553:LYS:HE2	1:A:573:GLU:HB2	1.87	0.55
1:A:178:THR:HG22	1:A:180:SER:OG	2.07	0.54
1:A:51:TRP:CZ3	1:A:114:PHE:HB2	2.42	0.54
1:A:224:MET:HG3	1:A:274:MET:HE1	1.88	0.54
1:A:306:THR:HG21	1:A:349:ARG:NH2	2.13	0.54
1:A:649:ASP:CB	1:A:653:ASN:HB2	2.37	0.54
1:A:410:ILE:HA	1:A:414:VAL:O	2.08	0.54
1:A:254:TRP:CE2	1:A:265:ASN:HB2	2.43	0.54
1:A:19:VAL:HG23	1:A:74:SER:OG	2.07	0.53
1:A:94:HIS:ND1	1:A:96:TYR:HB2	2.23	0.53
1:A:664:TYR:HB2	1:A:674:ILE:HD13	1.88	0.53
1:A:75:GLN:HA	1:A:131:ASP:O	2.08	0.53
1:A:416:VAL:HB	1:A:429:ALA:HA	1.90	0.53
1:A:138:SER:HB2	1:A:139:PRO:CD	2.38	0.53
1:A:615:ILE:HD12	1:A:615:ILE:N	2.24	0.53
1:A:204:ASP:OD1	1:A:208:LYS:NZ	2.36	0.52
1:A:411:ASN:CB	1:A:414:VAL:H	2.22	0.52
1:A:296:TRP:CG	1:A:415:TYR:HB2	2.45	0.52
1:A:9:PHE:CE2	1:A:129:ILE:HD11	2.45	0.52
1:A:22:PHE:HB3	3:A:700:HOH:O	2.10	0.52
1:A:138:SER:HB2	1:A:139:PRO:HD2	1.91	0.52
1:A:592:ASN:HB2	1:A:595:GLN:OE1	2.10	0.51
1:A:615:ILE:HG22	1:A:631:ILE:HD13	1.90	0.51
1:A:1:ALA:HB2	1:A:123:ALA:O	2.11	0.51
1:A:55:ILE:HG13	1:A:117:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:VAL:O	1:A:565:THR:HA	2.11	0.51
1:A:16:GLN:HG3	1:A:72:TRP:CD2	2.45	0.51
1:A:648:LYS:HG3	1:A:654:VAL:HG22	1.91	0.51
1:A:641:ILE:HG12	1:A:664:TYR:O	2.11	0.51
1:A:300:ASN:HD21	1:A:407:GLN:HB2	1.76	0.50
1:A:306:THR:HG23	1:A:349:ARG:HH21	1.73	0.50
1:A:593:LEU:CG	1:A:594:GLY:H	2.24	0.50
1:A:496:ILE:HG22	3:A:706:HOH:O	2.10	0.50
1:A:1:ALA:HB1	3:A:834:HOH:O	2.12	0.50
1:A:326:ASP:HB3	1:A:365:ASN:ND2	2.26	0.50
1:A:620:ASN:HD22	1:A:620:ASN:C	2.15	0.50
1:A:497:ILE:HD11	1:A:558:VAL:HG23	1.94	0.50
1:A:84:MET:HG2	1:A:85:ASN:H	1.77	0.49
1:A:397:ASN:ND2	1:A:487:ALA:HB1	2.26	0.49
1:A:227:VAL:CG1	1:A:254:TRP:HB2	2.42	0.49
1:A:18:VAL:HG13	1:A:356:TYR:CE1	2.47	0.49
1:A:137:THR:HG21	1:A:151:GLY:O	2.13	0.49
1:A:224:MET:HG3	1:A:274:MET:HE2	1.93	0.49
1:A:299:PHE:O	1:A:303:ILE:HG12	2.12	0.49
1:A:248:VAL:HG12	1:A:250:THR:HG22	1.95	0.49
1:A:122:HIS:HD2	3:A:766:HOH:O	1.95	0.49
1:A:258:GLU:CG	1:A:287:GLN:HE21	2.20	0.49
1:A:455:GLN:N	1:A:485:VAL:O	2.33	0.48
1:A:6:LYS:HG2	1:A:220:ASP:HA	1.96	0.48
1:A:23:VAL:O	1:A:49:GLY:HA2	2.13	0.48
1:A:283:GLN:HE21	1:A:283:GLN:CA	2.25	0.48
1:A:5:ASN:ND2	1:A:8:ASN:HB3	2.29	0.48
1:A:585:VAL:CB	1:A:675:ILE:HG12	2.40	0.48
1:A:57:LYS:HE2	1:A:377:PHE:CD1	2.48	0.47
1:A:542:ILE:C	1:A:542:ILE:HD13	2.35	0.47
1:A:486:TRP:HA	3:A:865:HOH:O	2.14	0.47
1:A:287:GLN:O	1:A:292:ASN:N	2.48	0.47
1:A:454:ASP:OD1	1:A:456:LEU:HB2	2.13	0.47
1:A:44:ARG:HG3	1:A:368:PRO:HG3	1.97	0.47
1:A:642:GLU:HA	1:A:662:HIS:O	2.14	0.47
1:A:438:TYR:O	1:A:477:ASP:HA	2.14	0.47
1:A:513:ILE:HD12	1:A:542:ILE:HD12	1.96	0.47
1:A:137:THR:HG23	1:A:138:SER:N	2.24	0.47
1:A:553:LYS:CD	1:A:573:GLU:HB2	2.45	0.46
1:A:639:LYS:NZ	3:A:831:HOH:O	2.43	0.46
1:A:606:LEU:HD11	1:A:633:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:THR:HA	1:A:537:TRP:CD1	2.51	0.46
1:A:615:ILE:HG21	1:A:633:VAL:HG22	1.97	0.46
1:A:374:MET:HG2	1:A:377:PHE:CZ	2.51	0.45
1:A:400:LEU:HD21	1:A:426:VAL:HG11	1.97	0.45
1:A:12:ASP:OD2	1:A:69:THR:HG22	2.15	0.45
1:A:230:MET:HE3	1:A:230:MET:HB2	1.67	0.45
1:A:522:THR:HA	1:A:537:TRP:CD2	2.51	0.45
1:A:375:SER:OG	1:A:376:SER:N	2.50	0.45
1:A:69:THR:O	1:A:126:ILE:HA	2.17	0.45
1:A:389:LYS:HE3	1:A:456:LEU:O	2.17	0.45
1:A:530:THR:HA	3:A:828:HOH:O	2.17	0.45
1:A:69:THR:HG23	3:A:688:HOH:O	2.16	0.45
1:A:294:ASP:OD1	1:A:295:ASN:N	2.46	0.45
1:A:326:ASP:HB3	1:A:365:ASN:HD22	1.81	0.45
1:A:184:ASP:O	1:A:188:ARG:HB2	2.17	0.44
1:A:223:ARG:HA	1:A:251:PHE:O	2.18	0.44
1:A:534:VAL:HA	1:A:544:VAL:HG23	1.98	0.44
1:A:17:ILE:HD11	1:A:71:ILE:HD11	1.99	0.44
1:A:425:VAL:O	1:A:488:TYR:N	2.45	0.44
1:A:488:TYR:CZ	1:A:490:ALA:HB2	2.52	0.44
1:A:242:ILE:HD13	1:A:250:THR:HG21	1.98	0.44
1:A:441:THR:HG22	1:A:475:ALA:HB2	1.99	0.44
1:A:262:ASP:OD1	1:A:264:ASN:N	2.48	0.44
1:A:657:GLU:OE2	1:A:662:HIS:NE2	2.34	0.44
1:A:270:ASN:HD21	1:A:310:TYR:HA	1.83	0.44
1:A:419:ARG:O	1:A:425:VAL:HA	2.18	0.44
1:A:526:LYS:O	1:A:556:ILE:HA	2.18	0.44
1:A:43:LEU:HD11	1:A:372:LYS:HA	1.99	0.43
1:A:44:ARG:HD2	1:A:88:SER:OG	2.18	0.43
1:A:420:GLN:HA	1:A:424:ASP:O	2.18	0.43
1:A:620:ASN:O	1:A:625:SER:HA	2.17	0.43
1:A:160:LEU:O	1:A:170:TYR:HE2	2.00	0.43
1:A:227:VAL:HG21	1:A:252:GLY:HA3	2.00	0.43
1:A:138:SER:CB	1:A:139:PRO:CD	2.96	0.43
1:A:59:ASN:N	1:A:59:ASN:HD22	2.15	0.43
1:A:514:ASP:OD1	1:A:541:GLN:HG3	2.19	0.43
1:A:20:ASP:OD2	1:A:47:CYS:N	2.46	0.42
1:A:533:ASN:O	1:A:544:VAL:HG22	2.19	0.42
1:A:142:GLU:OE1	1:A:173:HIS:HD2	2.02	0.42
1:A:266:HIS:CE1	1:A:280:ARG:NH2	2.85	0.42
1:A:649:ASP:OD1	1:A:653:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LEU:HA	1:A:448:PRO:HD3	1.89	0.42
1:A:513:ILE:O	1:A:541:GLN:HA	2.20	0.42
1:A:244:ASN:ND2	1:A:509:HIS:CE1	2.76	0.42
1:A:284:LYS:HE3	1:A:294:ASP:OD2	2.20	0.42
1:A:536:SER:O	1:A:542:ILE:HA	2.20	0.42
1:A:559:GLN:HB2	1:A:565:THR:OG1	2.20	0.42
1:A:518:PHE:HB2	1:A:539:ASN:CA	2.48	0.42
1:A:642:GLU:HG2	1:A:663:VAL:HG22	2.01	0.42
1:A:527:PHE:CZ	1:A:546:VAL:HG22	2.55	0.41
1:A:50:ASP:HB2	3:A:908:HOH:O	2.21	0.41
1:A:223:ARG:C	1:A:223:ARG:HD2	2.40	0.41
1:A:664:TYR:CD1	1:A:674:ILE:HD12	2.55	0.41
1:A:500:VAL:HB	1:A:503:MET:HE1	2.01	0.41
1:A:421:PHE:CE1	1:A:498:GLY:HA2	2.56	0.41
1:A:478:LEU:HD12	1:A:478:LEU:HA	1.80	0.41
1:A:542:ILE:HD11	1:A:544:VAL:HB	2.02	0.41
1:A:664:TYR:CE2	1:A:666:THR:HA	2.56	0.41
1:A:111:LEU:O	1:A:114:PHE:HB3	2.21	0.41
1:A:62:TYR:HD1	1:A:379:LYS:HE3	1.85	0.40
1:A:258:GLU:HA	1:A:283:GLN:HB3	2.03	0.40
1:A:236:LYS:HD2	1:A:504:MET:CE	2.51	0.40
1:A:593:LEU:HA	3:A:886:HOH:O	2.20	0.40
1:A:116:ARG:HH11	1:A:116:ARG:HD2	1.62	0.40
1:A:67:GLY:HA3	1:A:391:SER:OG	2.22	0.40
1:A:254:TRP:NE1	1:A:265:ASN:HB2	2.36	0.40
1:A:619:PHE:O	1:A:629:TRP:HA	2.21	0.40
1:A:620:ASN:HB2	1:A:626:TYR:HB2	2.03	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	678/680 (100%)	633 (93%)	41 (6%)	4 (1%)	25 43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	PHE
1	A	593	LEU
1	A	19	VAL
1	A	622	VAL

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	578/578 (100%)	481 (83%)	97 (17%)	2 4

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	LEU
1	A	11	SER
1	A	18	VAL
1	A	27	THR
1	A	38	SER
1	A	42	ASN
1	A	43	LEU
1	A	63	LEU
1	A	83	VAL
1	A	103	LYS
1	A	105	ASN
1	A	111	LEU
1	A	116	ARG
1	A	137	THR
1	A	143	THR
1	A	146	SER

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Mol	Chain	Res	Type
1	A	156	ASN
1	A	159	LEU
1	A	171	PHE
1	A	177	THR
1	A	178	THR
1	A	193	LEU
1	A	199	GLN
1	A	200	ASN
1	A	205	ARG
1	A	207	LEU
1	A	227	VAL
1	A	242	ILE
1	A	246	ARG
1	A	248	VAL
1	A	250	THR
1	A	256	LEU
1	A	257	SER
1	A	265	ASN
1	A	280	ARG
1	A	283	GLN
1	A	284	LYS
1	A	290	ARG
1	A	292	ASN
1	A	293	SER
1	A	306	THR
1	A	314	LEU
1	A	322	ASN
1	A	327	ARG
1	A	342	LEU
1	A	345	LEU
1	A	346	LEU
1	A	349	ARG
1	A	368	PRO
1	A	371	ARG
1	A	381	THR
1	A	386	VAL
1	A	393	LEU
1	A	405	THR
1	A	406	GLU
1	A	407	GLN
1	A	409	TRP
1	A	411	ASN

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Mol	Chain	Res	Type
1	A	416	VAL
1	A	425	VAL
1	A	426	VAL
1	A	428	VAL
1	A	430	VAL
1	A	437	ASN
1	A	459	LEU
1	A	463	ASN
1	A	477	ASP
1	A	482	GLU
1	A	493	SER
1	A	510	GLN
1	A	520	THR
1	A	522	THR
1	A	524	THR
1	A	529	THR
1	A	542	ILE
1	A	543	VAL
1	A	544	VAL
1	A	550	SER
1	A	561	SER
1	A	562	SER
1	A	580	VAL
1	A	583	ARG
1	A	592	ASN
1	A	593	LEU
1	A	600	VAL
1	A	602	ASN
1	A	603	VAL
1	A	606	LEU
1	A	620	ASN
1	A	635	VAL
1	A	639	LYS
1	A	649	ASP
1	A	658	SER
1	A	660	SER
1	A	668	THR
1	A	669	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	56	ASN
1	A	59	ASN
1	A	79	ASN
1	A	105	ASN
1	A	122	HIS
1	A	156	ASN
1	A	165	ASN
1	A	173	HIS
1	A	200	ASN
1	A	235	GLN
1	A	270	ASN
1	A	283	GLN
1	A	291	ASN
1	A	300	ASN
1	A	304	GLN
1	A	365	ASN
1	A	388	GLN
1	A	396	ASN
1	A	397	ASN
1	A	474	ASN
1	A	509	HIS
1	A	510	GLN
1	A	521	ASN
1	A	533	ASN
1	A	539	ASN
1	A	540	ASN
1	A	559	GLN
1	A	577	ASN
1	A	579	GLN
1	A	602	ASN
1	A	608	ASN
1	A	620	ASN
1	A	651	GLN
1	A	653	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 2 ligands modelled in this entry, 2 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	680/680 (100%)	-0.67	1 (0%)	95	96	6, 12, 21, 34	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	3.6

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	681	1/1	0.98	0.06	9,9,9,9	0
2	CA	A	682	1/1	0.99	0.12	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.