Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:25 AM GMT

PDB ID	:	3OY2
Title	:	Crystal structure of a putative glycosyltransferase from Paramecium bursaria Chlorella virus NY2A
Authors	:	Xiang, Y.; Rossmann, M.G.
Deposited on	:	2010-09-22
Resolution	:	2.31 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

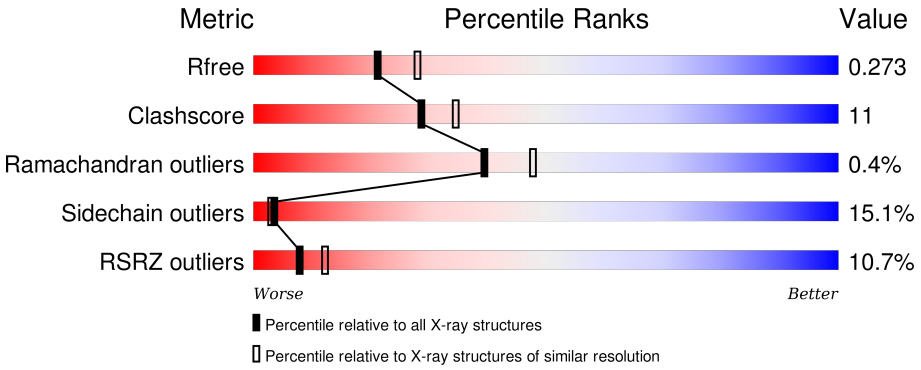
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.31 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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	413	2% 69% 17% 7% • 5%
1	B	413	18% 67% 21% 7% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6309 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 Glycosyltransferase B736L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3101	1983	531	568	19			
1	B	392	Total	C	N	O	S	0	0	0
			3101	1983	531	568	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	LEU	-	EXPRESSION TAG	UNP A7IXR1
A	407	GLU	-	EXPRESSION TAG	UNP A7IXR1
A	408	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	409	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	410	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	411	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	412	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	413	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	406	LEU	-	EXPRESSION TAG	UNP A7IXR1
B	407	GLU	-	EXPRESSION TAG	UNP A7IXR1
B	408	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	409	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	410	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	411	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	412	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	413	HIS	-	EXPRESSION TAG	UNP A7IXR1

- Molecule 2 is water.

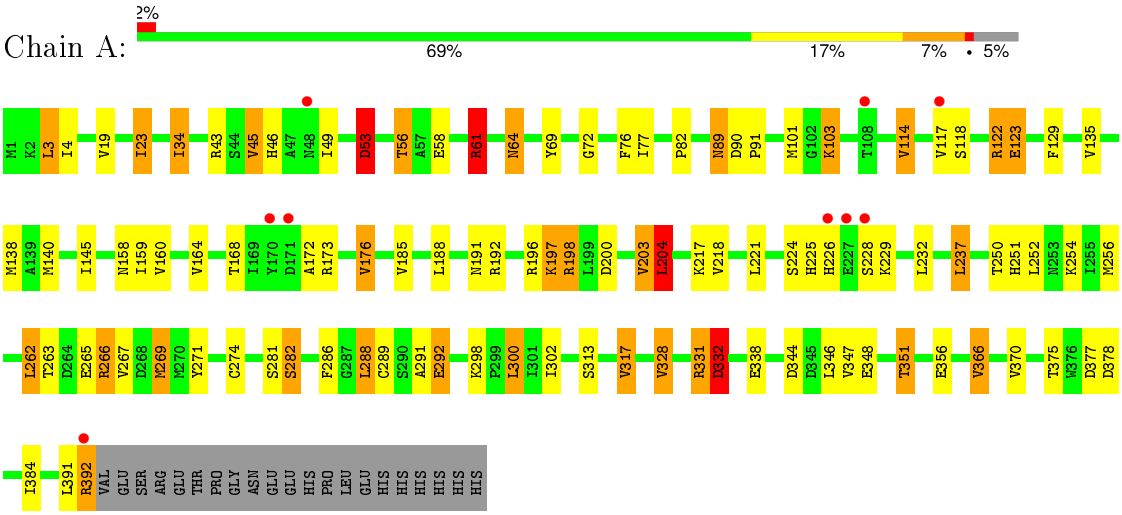
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	37	Total	O	0	0
			37	37		

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 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.

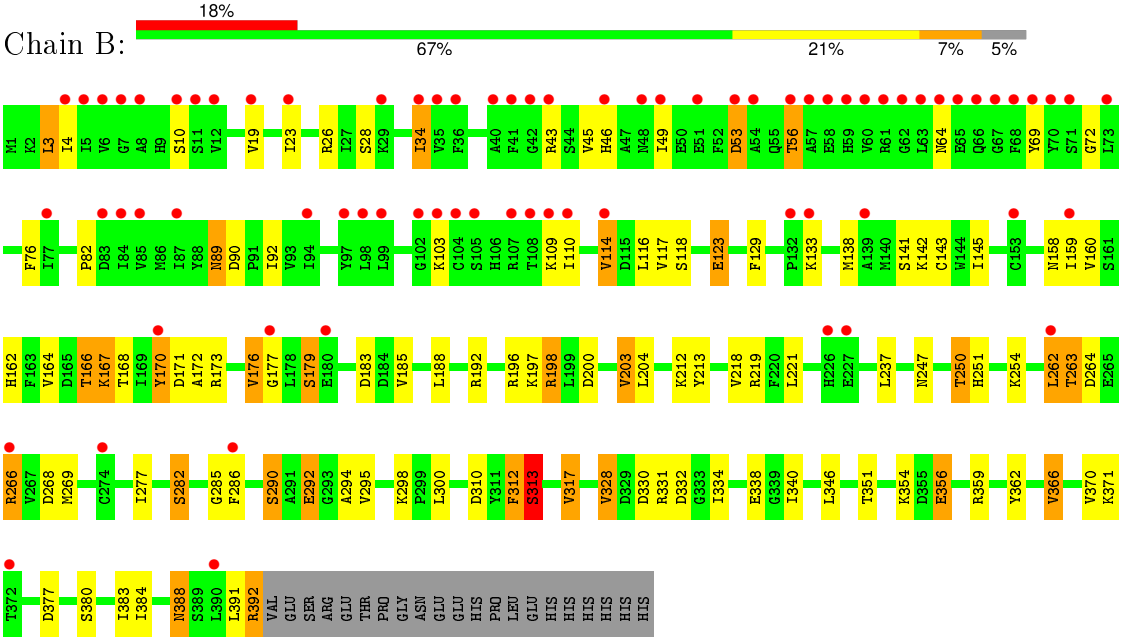
- Molecule 1: Glycosyltransferase B736L

Chain A:



- Molecule 1: Glycosyltransferase B736L

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	153.62Å 246.94Å 67.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.19 – 2.31 47.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (130.19-2.31) 99.4 (47.02-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.45 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.233 , 0.268 0.241 , 0.273	Depositor DCC
R_{free} test set	2843 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 56077 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6309	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.82	4/3168 (0.1%)	0.97	13/4284 (0.3%)
1	B	0.72	1/3168 (0.0%)	0.88	5/4284 (0.1%)
All	All	0.77	5/6336 (0.1%)	0.92	18/8568 (0.2%)

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	1
1	B	0	3
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	ASN	CB-CG	12.44	1.79	1.51
1	A	328	VAL	CB-CG1	-6.58	1.39	1.52
1	A	332	ASP	CB-CG	-5.74	1.39	1.51
1	A	274	CYS	CB-SG	5.40	1.91	1.82
1	A	218	VAL	CB-CG2	-5.06	1.42	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	198	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	A	198	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	B	198	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	196	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	332	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	B	203	VAL	CG1-CB-CG2	6.52	121.33	110.90
1	A	122	ARG	NE-CZ-NH1	6.47	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3	LEU	CA-CB-CG	6.29	129.76	115.30
1	B	340	ILE	CG1-CB-CG2	-5.71	98.84	111.40
1	A	332	ASP	CB-CA-C	-5.51	99.37	110.40
1	A	3	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	300	LEU	CB-CG-CD1	-5.44	101.76	111.00
1	A	196	ARG	CG-CD-NE	-5.21	100.85	111.80
1	A	122	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	328	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	A	204	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	61	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	53	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	ARG	Peptide
1	B	262	LEU	Peptide
1	B	312	PHE	Peptide
1	B	331	ARG	Peptide

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	3101	0	3089	81	0
1	B	3101	0	3089	64	0
2	A	70	0	0	7	0
2	B	37	0	0	5	0
All	All	6309	0	6178	142	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 11.

All (142) 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:B:388:ASN:CG	1:B:388:ASN:CB	1.79	1.46
1:A:262:LEU:O	1:A:262:LEU:HG	1.55	1.05
1:B:34:ILE:HD11	1:B:76:PHE:HZ	1.22	1.05
1:A:229:LYS:HE3	1:B:330:ASP:HB2	1.39	1.02
1:B:34:ILE:HD11	1:B:76:PHE:CZ	1.98	0.99
1:A:34:ILE:HD11	1:A:76:PHE:HZ	1.26	0.98
1:A:262:LEU:O	1:A:262:LEU:CG	2.11	0.96
1:A:34:ILE:HD11	1:A:76:PHE:CZ	2.03	0.94
1:A:191:ASN:HB3	1:A:197:LYS:HG2	1.50	0.94
1:A:344:ASP:O	1:A:348:GLU:HG3	1.77	0.84
1:A:53:ASP:OD1	1:A:56:THR:HG23	1.77	0.84
1:B:19:VAL:O	1:B:23:ILE:HG22	1.79	0.82
1:B:266:ARG:HH11	1:B:266:ARG:HG3	1.45	0.82
1:B:392:ARG:HA	1:B:392:ARG:HE	1.46	0.81
1:A:138:MET:HE1	1:A:160:VAL:HG21	1.63	0.80
1:A:123:GLU:HG2	1:B:237:LEU:HD22	1.64	0.79
1:B:53:ASP:OD1	1:B:56:THR:HG23	1.83	0.78
1:A:64:ASN:HB2	2:A:434:HOH:O	1.86	0.76
1:B:300:LEU:HB2	1:B:317:VAL:HG22	1.69	0.74
1:B:164:VAL:HG21	1:B:292:GLU:HA	1.70	0.74
1:A:331:ARG:HD3	2:A:436:HOH:O	1.87	0.73
1:A:103:LYS:HB2	2:A:458:HOH:O	1.88	0.72
1:A:262:LEU:CD1	1:A:262:LEU:O	2.37	0.72
1:A:19:VAL:O	1:A:23:ILE:HG22	1.89	0.72
1:A:53:ASP:OD1	1:A:56:THR:CG2	2.38	0.70
1:A:328:VAL:HG11	1:A:331:ARG:CZ	2.21	0.70
1:A:262:LEU:HD12	1:A:262:LEU:O	1.92	0.70
1:A:391:LEU:O	1:A:392:ARG:HB2	1.89	0.70
1:A:328:VAL:O	1:A:328:VAL:HG12	1.90	0.69
1:A:138:MET:CE	1:A:160:VAL:HG21	2.23	0.69
1:A:300:LEU:HB2	1:A:317:VAL:HG22	1.73	0.69
1:A:138:MET:HE1	1:A:160:VAL:CG2	2.23	0.69
1:A:262:LEU:HB2	1:A:267:VAL:HG23	1.77	0.67
1:A:328:VAL:HG13	1:A:331:ARG:HG3	1.75	0.67
1:A:176:VAL:HG13	1:A:269:MET:HB3	1.76	0.66
1:A:251:HIS:HD2	1:A:254:LYS:NZ	1.95	0.65
1:B:219:ARG:NH1	2:B:443:HOH:O	2.31	0.64
1:A:237:LEU:HD13	1:B:123:GLU:HG2	1.80	0.63
1:B:247:ASN:HB3	1:B:250:THR:HG23	1.81	0.63
1:A:138:MET:CE	1:A:160:VAL:CG2	2.77	0.63
1:B:138:MET:HE1	1:B:160:VAL:HG21	1.80	0.62
1:A:286:PHE:HB3	1:A:288:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:HB	1:B:300:LEU:CD2	2.30	0.61
1:A:191:ASN:CB	1:A:197:LYS:HG2	2.27	0.61
1:B:170:TYR:CD2	1:B:171:ASP:HB2	2.36	0.61
1:B:282:SER:HB3	1:B:338:GLU:OE1	2.01	0.61
1:A:282:SER:HB3	1:A:338:GLU:OE1	2.00	0.60
1:B:53:ASP:OD1	1:B:56:THR:CG2	2.50	0.59
1:B:145:ILE:HD11	1:B:159:ILE:HD11	1.84	0.59
1:B:277:ILE:HB	1:B:300:LEU:HD23	1.83	0.59
1:B:138:MET:CE	1:B:160:VAL:HG21	2.32	0.59
1:A:135:VAL:HG11	2:A:445:HOH:O	2.03	0.59
1:A:225:HIS:CE1	1:A:228:SER:HB2	2.38	0.58
1:A:145:ILE:HD11	1:A:159:ILE:HD11	1.86	0.58
1:A:375:THR:CG2	1:A:378:ASP:H	2.17	0.57
1:B:89:ASN:HD22	1:B:90:ASP:H	1.53	0.57
1:A:225:HIS:NE2	1:A:228:SER:HB2	2.19	0.56
1:A:347:VAL:O	1:A:351:THR:HG22	2.05	0.56
1:B:114:VAL:HG21	1:B:129:PHE:HE2	1.71	0.56
1:A:45:VAL:HG12	1:A:46:HIS:CD2	2.40	0.56
1:A:375:THR:HG22	1:A:378:ASP:H	1.71	0.55
1:A:375:THR:HG22	1:A:378:ASP:CG	2.27	0.54
1:B:4:ILE:HD12	1:B:82:PRO:HG3	1.89	0.54
1:A:192:ARG:HH11	1:A:192:ARG:HG2	1.71	0.54
1:A:122:ARG:NH2	1:A:332:ASP:O	2.41	0.53
1:A:53:ASP:CG	1:A:56:THR:HG23	2.30	0.53
1:B:263:THR:OG1	1:B:266:ARG:HG2	2.09	0.53
1:B:143:CYS:HB3	1:B:310:ASP:OD2	2.08	0.52
1:A:328:VAL:CG1	1:A:331:ARG:HG3	2.38	0.52
1:A:176:VAL:CG1	1:A:269:MET:HB3	2.39	0.52
1:B:172:ALA:O	1:B:176:VAL:HG22	2.09	0.52
1:B:28:SER:HB3	2:B:426:HOH:O	2.08	0.52
1:A:4:ILE:HD12	1:A:82:PRO:HG3	1.92	0.52
1:A:114:VAL:HG21	1:A:129:PHE:HE2	1.75	0.52
1:B:388:ASN:CA	1:B:388:ASN:CG	2.71	0.51
1:B:251:HIS:HD2	1:B:254:LYS:NZ	2.07	0.51
1:A:251:HIS:HD2	1:A:254:LYS:HZ2	1.57	0.51
1:A:89:ASN:HD22	1:A:90:ASP:H	1.58	0.51
1:A:251:HIS:CD2	1:A:254:LYS:NZ	2.79	0.51
1:B:196:ARG:O	1:B:282:SER:HB2	2.11	0.51
1:B:166:THR:HG22	1:B:268:ASP:OD2	2.12	0.49
1:A:200:ASP:O	1:A:204:LEU:HB2	2.13	0.49
1:B:380:SER:O	1:B:384:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:HIS:HD2	1:B:254:LYS:HZ2	1.61	0.48
1:B:328:VAL:O	1:B:328:VAL:CG1	2.61	0.47
1:B:388:ASN:CB	1:B:388:ASN:ND2	2.67	0.47
1:A:328:VAL:HG11	1:A:331:ARG:NH1	2.29	0.47
1:A:138:MET:HA	1:A:158:ASN:O	2.14	0.47
1:B:167:LYS:NZ	1:B:167:LYS:HB2	2.28	0.47
1:B:198:ARG:HD3	1:B:200:ASP:OD1	2.15	0.46
1:A:263:THR:OG1	1:A:266:ARG:HG2	2.15	0.46
1:A:69:TYR:CE2	1:A:72:GLY:HA3	2.50	0.46
1:A:203:VAL:HG21	1:A:232:LEU:HB3	1.98	0.46
1:B:312:PHE:O	1:B:313:SER:HB2	2.15	0.46
1:B:138:MET:HE1	1:B:160:VAL:CG2	2.46	0.45
1:B:92:ILE:HG13	1:B:334:ILE:HG22	1.97	0.45
1:B:138:MET:CE	1:B:160:VAL:CG2	2.94	0.45
1:B:116:LEU:O	1:B:285:GLY:HA2	2.16	0.45
1:B:179:SER:HB2	2:B:444:HOH:O	2.15	0.45
1:A:77:ILE:HD13	1:A:101:MET:HE3	1.99	0.45
1:A:266:ARG:HA	1:A:269:MET:HE2	1.98	0.45
1:B:26:ARG:HD3	1:B:377:ASP:OD1	2.16	0.45
1:A:262:LEU:HB2	1:A:267:VAL:CG2	2.46	0.45
1:B:290:SER:C	1:B:292:GLU:N	2.69	0.44
1:A:172:ALA:O	1:A:176:VAL:HG22	2.17	0.44
1:A:198:ARG:HD3	1:A:200:ASP:OD1	2.17	0.44
1:B:356:GLU:HB3	1:B:359:ARG:NH2	2.32	0.44
1:A:251:HIS:CD2	1:A:254:LYS:HZ1	2.36	0.44
1:B:212:LYS:HG2	1:B:213:TYR:CE1	2.52	0.44
1:B:294:ALA:HB2	1:B:300:LEU:HD11	2.00	0.44
1:B:362:TYR:O	1:B:366:VAL:HG22	2.17	0.44
1:A:302:ILE:O	1:A:302:ILE:HG13	2.17	0.44
1:B:110:ILE:HD12	1:B:133:LYS:HB2	2.00	0.44
1:A:135:VAL:HG13	2:A:451:HOH:O	2.18	0.43
1:B:109:LYS:HE2	1:B:391:LEU:HD23	2.00	0.43
1:B:166:THR:OG1	1:B:292:GLU:O	2.34	0.43
1:B:183:ASP:HB2	2:B:435:HOH:O	2.17	0.43
1:A:317:VAL:HG23	1:A:366:VAL:HG13	2.01	0.43
1:A:375:THR:HG23	1:A:377:ASP:N	2.33	0.43
1:A:392:ARG:NE	1:A:392:ARG:HA	2.34	0.43
1:B:53:ASP:CG	1:B:56:THR:HG23	2.40	0.43
1:A:90:ASP:HB2	1:A:91:PRO:CD	2.49	0.43
1:B:138:MET:HA	1:B:158:ASN:O	2.19	0.42
1:A:197:LYS:HA	1:A:281:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:THR:OG1	1:A:266:ARG:CG	2.68	0.42
1:B:177:GLY:HA2	2:B:444:HOH:O	2.18	0.42
1:A:271:TYR:CZ	1:A:292:GLU:HG3	2.54	0.42
1:A:328:VAL:O	1:A:328:VAL:CG1	2.65	0.42
1:A:61:ARG:NH2	2:A:454:HOH:O	2.48	0.42
1:A:23:ILE:HG21	1:A:23:ILE:HD13	1.66	0.42
1:A:347:VAL:O	1:A:351:THR:CG2	2.68	0.41
1:A:140:MET:HE1	2:A:423:HOH:O	2.20	0.41
1:A:176:VAL:HG13	1:A:269:MET:HE3	2.01	0.41
1:B:164:VAL:CG2	1:B:292:GLU:HA	2.46	0.41
1:A:118:SER:OG	1:A:338:GLU:OE2	2.31	0.41
1:B:10:SER:HB3	1:B:45:VAL:HB	2.03	0.41
1:B:370:VAL:HG12	1:B:370:VAL:O	2.20	0.41
1:B:45:VAL:HG12	1:B:46:HIS:CD2	2.55	0.41
1:A:286:PHE:HB3	1:A:288:LEU:CD2	2.51	0.40
1:B:162:HIS:HB2	1:B:286:PHE:CZ	2.56	0.40
1:B:69:TYR:CE2	1:B:72:GLY:HA3	2.56	0.40
1:A:164:VAL:HG21	1:A:292:GLU:HA	2.02	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	390/413 (94%)	379 (97%)	10 (3%)	1 (0%)	46	56
1	B	390/413 (94%)	376 (96%)	12 (3%)	2 (0%)	34	40
All	All	780/826 (94%)	755 (97%)	22 (3%)	3 (0%)	39	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	313	SER
1	B	290	SER
1	A	291	ALA

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	341/361 (94%)	290 (85%)	51 (15%)	3 3
1	B	341/361 (94%)	289 (85%)	52 (15%)	3 3
All	All	682/722 (94%)	579 (85%)	103 (15%)	3 3

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	23	ILE
1	A	34	ILE
1	A	43	ARG
1	A	45	VAL
1	A	49	ILE
1	A	53	ASP
1	A	56	THR
1	A	58	GLU
1	A	61	ARG
1	A	64	ASN
1	A	89	ASN
1	A	103	LYS
1	A	114	VAL
1	A	117	VAL
1	A	123	GLU
1	A	168	THR
1	A	173	ARG
1	A	176	VAL
1	A	185	VAL
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	197	LYS
1	A	203	VAL
1	A	204	LEU
1	A	217	LYS
1	A	221	LEU
1	A	224	SER
1	A	226	HIS
1	A	237	LEU
1	A	250	THR
1	A	252	LEU
1	A	256	MET
1	A	262	LEU
1	A	265	GLU
1	A	266	ARG
1	A	269	MET
1	A	282	SER
1	A	288	LEU
1	A	289	CYS
1	A	292	GLU
1	A	298	LYS
1	A	313	SER
1	A	317	VAL
1	A	332	ASP
1	A	346	LEU
1	A	351	THR
1	A	356	GLU
1	A	366	VAL
1	A	370	VAL
1	A	384	ILE
1	A	392	ARG
1	B	3	LEU
1	B	34	ILE
1	B	43	ARG
1	B	49	ILE
1	B	53	ASP
1	B	56	THR
1	B	64	ASN
1	B	89	ASN
1	B	103	LYS
1	B	114	VAL
1	B	117	VAL
1	B	118	SER

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Mol	Chain	Res	Type
1	B	123	GLU
1	B	141	SER
1	B	142	LYS
1	B	166	THR
1	B	167	LYS
1	B	168	THR
1	B	170	TYR
1	B	173	ARG
1	B	176	VAL
1	B	179	SER
1	B	185	VAL
1	B	188	LEU
1	B	192	ARG
1	B	197	LYS
1	B	203	VAL
1	B	204	LEU
1	B	218	VAL
1	B	221	LEU
1	B	250	THR
1	B	262	LEU
1	B	263	THR
1	B	264	ASP
1	B	266	ARG
1	B	269	MET
1	B	282	SER
1	B	292	GLU
1	B	295	VAL
1	B	298	LYS
1	B	313	SER
1	B	317	VAL
1	B	328	VAL
1	B	332	ASP
1	B	346	LEU
1	B	351	THR
1	B	354	LYS
1	B	356	GLU
1	B	366	VAL
1	B	371	LYS
1	B	383	ILE
1	B	392	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	46	HIS
1	A	59	HIS
1	A	89	ASN
1	A	131	HIS
1	A	162	HIS
1	A	251	HIS
1	B	46	HIS
1	B	55	GLN
1	B	89	ASN
1	B	225	HIS
1	B	251	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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	392/413 (94%)	0.22	9 (2%) 64 72	27, 43, 67, 88	0
1	B	392/413 (94%)	1.02	75 (19%) 2 2	27, 72, 151, 192	0
All	All	784/826 (94%)	0.62	84 (10%) 8 12	27, 51, 136, 192	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	LEU	9.8
1	B	60	VAL	8.8
1	B	69	TYR	8.1
1	B	63	LEU	7.6
1	B	41	PHE	5.5
1	B	36	PHE	5.4
1	B	262	LEU	5.3
1	B	64	ASN	5.3
1	A	226	HIS	5.2
1	B	43	ARG	5.2
1	B	108	THR	4.9
1	A	227	GLU	4.7
1	B	56	THR	4.7
1	B	390	LEU	4.5
1	B	40	ALA	4.5
1	B	132	PRO	4.5
1	B	70	TYR	4.4
1	B	12	VAL	4.4
1	B	49	ILE	4.4
1	B	61	ARG	4.2
1	B	71	SER	4.0
1	B	109	LYS	3.9
1	B	105	SER	3.9
1	B	133	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	103	LYS	3.8
1	B	286	PHE	3.8
1	B	226	HIS	3.7
1	B	8	ALA	3.7
1	A	170	TYR	3.6
1	B	62	GLY	3.5
1	B	98	LEU	3.5
1	B	51	GLU	3.3
1	B	97	TYR	3.3
1	B	42	GLY	3.2
1	B	67	GLY	3.1
1	B	7	GLY	3.1
1	B	57	ALA	3.1
1	B	73	LEU	3.1
1	B	54	ALA	3.0
1	B	4	ILE	3.0
1	B	170	TYR	3.0
1	B	48	ASN	2.9
1	B	139	ALA	2.9
1	B	66	GLN	2.9
1	B	94	ILE	2.9
1	B	84	ILE	2.8
1	B	104	CYS	2.8
1	B	46	HIS	2.8
1	B	83	ASP	2.7
1	B	19	VAL	2.7
1	B	5	ILE	2.7
1	A	171	ASP	2.7
1	B	23	ILE	2.7
1	B	68	PHE	2.7
1	B	85	VAL	2.6
1	B	87	ILE	2.6
1	A	108	THR	2.6
1	B	35	VAL	2.6
1	B	102	GLY	2.5
1	B	177	GLY	2.5
1	B	159	ILE	2.5
1	B	58	GLU	2.5
1	B	65	GLU	2.4
1	B	29	LYS	2.4
1	B	107	ARG	2.4
1	B	53	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	59	HIS	2.3
1	B	266	ARG	2.3
1	B	11	SER	2.3
1	B	114	VAL	2.3
1	A	117	VAL	2.3
1	B	6	VAL	2.3
1	B	372	THR	2.3
1	B	77	ILE	2.2
1	A	48	ASN	2.2
1	B	110	ILE	2.2
1	B	227	GLU	2.2
1	A	392	ARG	2.2
1	B	153	CYS	2.2
1	B	274	CYS	2.2
1	B	180	GLU	2.2
1	B	34	ILE	2.1
1	B	10	SER	2.1
1	A	228	SER	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.