Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:13 PM GMT

PDB ID	:	1JDA
Title	:	MALTOTETRAOSE-FORMING EXO-AMYLASE
Authors	:	Yoshioka, Y.; Hasegawa, K.; Matsuura, Y.; Katsube, Y.; Kubota, M.
Deposited on	:	1997-06-16
Resolution	:	2.20 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:

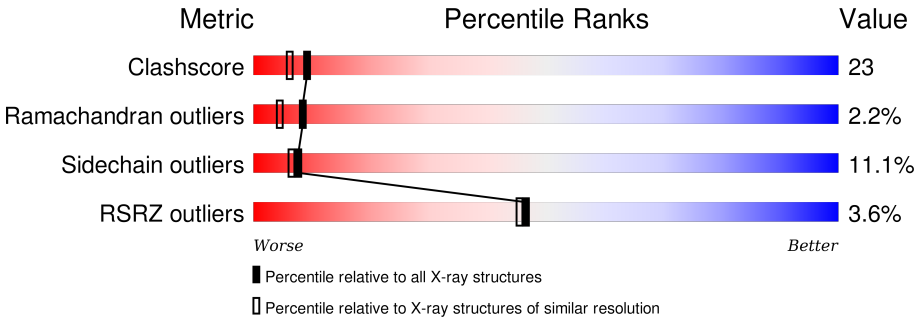
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	429	3%, 55%, 31%, 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3502 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 1,4-ALPHA MALTOTETRAHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3297	2070	597	620	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLN	GLU	ENGINEERED	UNP P13507
A	334	ASP	SER	CONFLICT	UNP P13507

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

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

- Molecule 3 is water.

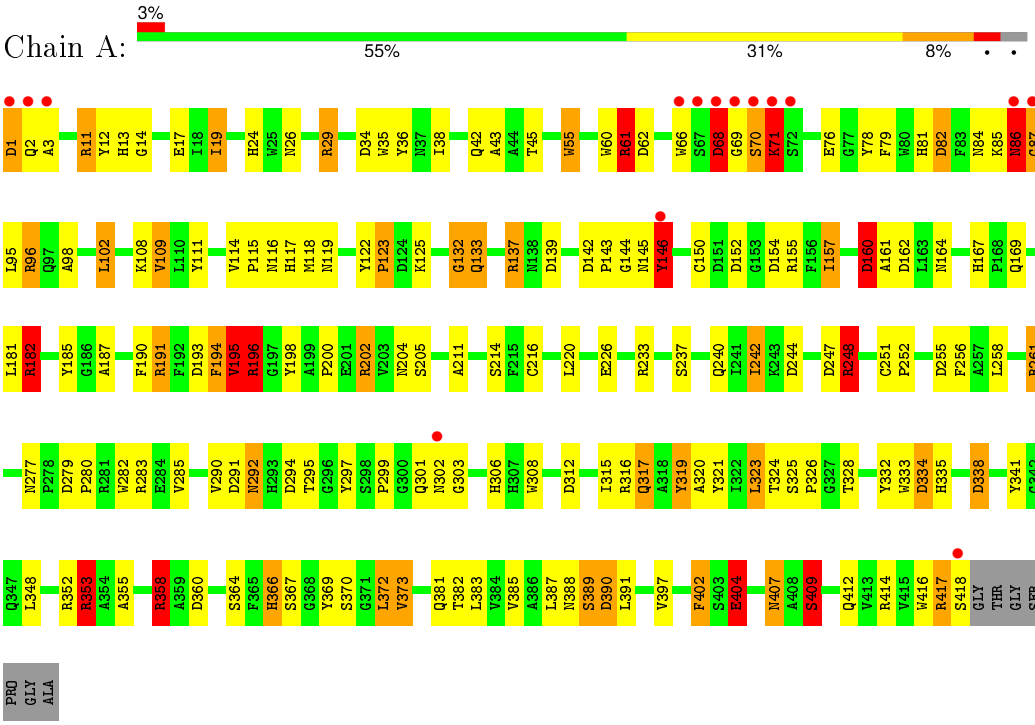
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		

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: 1,4-ALPHA MALTOTETRAHYDROLASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.70Å 171.00Å 46.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 32.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 96.0 (32.26-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.77 (at 2.20Å)	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.174 , (Not available) 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 26550 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3502	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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

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	1.14	3/3402 (0.1%)	2.25	104/4631 (2.2%)

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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	ARG	CD-NE	-6.04	1.36	1.46
1	A	248	ARG	NE-CZ	-5.50	1.25	1.33
1	A	353	ARG	CZ-NH2	5.18	1.39	1.33

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	ARG	CD-NE-CZ	38.22	177.11	123.60
1	A	346	ARG	NE-CZ-NH1	25.66	133.13	120.30
1	A	196	ARG	NE-CZ-NH1	23.76	132.18	120.30
1	A	11	ARG	NE-CZ-NH1	23.76	132.18	120.30
1	A	248	ARG	NE-CZ-NH1	21.05	130.82	120.30
1	A	29	ARG	NE-CZ-NH1	20.92	130.76	120.30
1	A	29	ARG	CD-NE-CZ	19.30	150.62	123.60
1	A	358	ARG	NE-CZ-NH1	19.15	129.88	120.30
1	A	283	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	A	353	ARG	NE-CZ-NH1	16.91	128.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	NE-CZ-NH1	16.61	128.60	120.30
1	A	182	ARG	NE-CZ-NH2	-15.81	112.39	120.30
1	A	196	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	A	182	ARG	NE-CZ-NH1	13.19	126.89	120.30
1	A	146	TYR	CB-CA-C	12.81	136.02	110.40
1	A	82	ASP	CB-CG-OD1	-12.80	106.78	118.30
1	A	414	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	A	414	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	A	34	ASP	CB-CG-OD1	12.21	129.29	118.30
1	A	61	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	A	175	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	A	346	ARG	CD-NE-CZ	11.02	139.02	123.60
1	A	390	ASP	CB-CG-OD1	10.94	128.15	118.30
1	A	191	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	137	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	A	353	ARG	CD-NE-CZ	9.95	137.53	123.60
1	A	146	TYR	CA-CB-CG	9.26	131.00	113.40
1	A	196	ARG	CD-NE-CZ	9.16	136.42	123.60
1	A	247	ASP	CB-CG-OD1	8.62	126.05	118.30
1	A	346	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	82	ASP	CB-CA-C	-8.39	93.61	110.40
1	A	194	PHE	C-N-CA	8.39	142.68	121.70
1	A	360	ASP	CB-CG-OD1	8.34	125.81	118.30
1	A	358	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	353	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	A	366	HIS	C-N-CA	8.17	142.12	121.70
1	A	338	ASP	CB-CG-OD2	8.13	125.62	118.30
1	A	248	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	242	ILE	CA-CB-CG2	8.11	127.11	110.90
1	A	346	ARG	NH1-CZ-NH2	-8.05	110.54	119.40
1	A	11	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	297	TYR	CB-CG-CD1	7.90	125.74	121.00
1	A	417	ARG	C-N-CA	7.76	141.10	121.70
1	A	255	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	416	TRP	C-N-CA	7.68	140.90	121.70
1	A	152	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	29	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	139	ASP	CB-CG-OD2	7.53	125.08	118.30
1	A	160	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	417	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	233	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	A	11	ARG	NH1-CZ-NH2	-7.44	111.22	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	390	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	316	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	92	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	414	ARG	CD-NE-CZ	6.89	133.24	123.60
1	A	409	SER	N-CA-CB	6.62	120.43	110.50
1	A	324	THR	CA-CB-CG2	6.59	121.63	112.40
1	A	62	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	68	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	29	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	A	1	ASP	CB-CG-OD1	-6.37	112.56	118.30
1	A	358	ARG	CD-NE-CZ	6.34	132.47	123.60
1	A	369	TYR	CA-CB-CG	-6.20	101.63	113.40
1	A	343	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	261	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	175	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
1	A	86	ASN	C-N-CA	5.91	134.71	122.30
1	A	248	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
1	A	334	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	98	ALA	CB-CA-C	5.85	118.88	110.10
1	A	96	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	139	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	A	269	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	242	ILE	CB-CA-C	5.72	123.04	111.60
1	A	175	ARG	CD-NE-CZ	5.70	131.57	123.60
1	A	96	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	A	297	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	A	372	LEU	CA-CB-CG	5.62	128.24	115.30
1	A	226	GLU	OE1-CD-OE2	5.62	130.05	123.30
1	A	181	LEU	CB-CA-C	5.62	120.87	110.20
1	A	142	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	185	TYR	C-N-CA	5.61	134.08	122.30
1	A	45	THR	CA-CB-CG2	5.48	120.08	112.40
1	A	202	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	402	PHE	C-N-CA	5.46	135.34	121.70
1	A	338	ASP	O-C-N	5.44	131.40	122.70
1	A	319	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	177	GLU	CG-CD-OE1	5.42	129.13	118.30
1	A	160	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	256	PHE	N-CA-CB	5.39	120.30	110.60
1	A	92	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	195	VAL	CG1-CB-CG2	5.21	119.24	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	PHE	O-C-N	5.19	131.00	122.70
1	A	55	TRP	CA-CB-CG	5.10	123.40	113.70
1	A	291	ASP	N-CA-CB	5.09	119.76	110.60
1	A	181	LEU	N-CA-CB	-5.07	100.25	110.40
1	A	404	GLU	CA-CB-CG	5.07	124.55	113.40
1	A	341	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	36	TYR	CB-CG-CD1	5.06	124.04	121.00
1	A	109	VAL	CA-CB-CG1	5.04	118.47	110.90
1	A	251	CYS	CB-CA-C	-5.03	100.34	110.40
1	A	291	ASP	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	A	353	ARG	Sidechain

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	3297	0	3011	145	0
2	A	2	0	0	0	0
3	A	203	0	0	12	0
All	All	3502	0	3011	145	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 (145) 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:370:SER:O	1:A:389:SER:HB2	1.24	1.24
1:A:71:LYS:HD3	1:A:302:ASN:OD1	1.61	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:HD22	1:A:279:ASP:H	1.07	1.01
1:A:370:SER:O	1:A:389:SER:CB	2.10	0.99
1:A:145:ASN:HD21	1:A:154:ASP:HB3	1.24	0.98
1:A:116:ASN:HD22	1:A:117:HIS:HD2	1.06	0.98
1:A:334:ASP:OD1	1:A:338:ASP:OD2	1.87	0.92
1:A:11:ARG:HH22	1:A:204:ASN:ND2	1.68	0.92
1:A:11:ARG:HH12	1:A:204:ASN:HD22	0.92	0.91
1:A:299:PRO:HD3	1:A:334:ASP:OD2	1.70	0.91
1:A:11:ARG:HH12	1:A:204:ASN:ND2	1.68	0.90
1:A:86:ASN:OD1	1:A:86:ASN:C	2.11	0.89
1:A:17:GLU:OE2	1:A:108:LYS:HE2	1.74	0.87
1:A:11:ARG:NH1	1:A:204:ASN:HD22	1.70	0.87
1:A:26:ASN:HD22	1:A:29:ARG:HH11	1.26	0.82
1:A:61:ARG:HD2	1:A:84:ASN:HB3	1.60	0.82
1:A:70:SER:O	1:A:71:LYS:HB2	1.79	0.79
1:A:116:ASN:HD22	1:A:117:HIS:CD2	1.96	0.79
1:A:277:ASN:ND2	1:A:279:ASP:H	1.79	0.79
1:A:211:ALA:HB1	1:A:214:SER:OG	1.83	0.78
1:A:143:PRO:HB2	1:A:146:TYR:HE1	1.48	0.78
1:A:409:SER:O	1:A:412:GLN:HG3	1.84	0.78
1:A:132:GLY:O	1:A:133:GLN:HG2	1.84	0.77
1:A:160:ASP:N	1:A:160:ASP:OD1	2.14	0.77
1:A:317:GLN:HE21	1:A:317:GLN:H	1.31	0.76
1:A:145:ASN:HD21	1:A:154:ASP:CB	2.01	0.73
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.21	0.73
1:A:86:ASN:OD1	1:A:87:GLY:N	2.22	0.73
1:A:319:TYR:OH	1:A:335:HIS:CD2	2.42	0.73
1:A:216:CYS:O	1:A:252:PRO:HD2	1.88	0.73
1:A:24:HIS:HD2	1:A:26:ASN:H	1.38	0.72
1:A:292:ASN:ND2	1:A:294:ASP:H	1.89	0.70
1:A:358:ARG:HG3	3:A:530:HOH:O	1.91	0.69
1:A:82:ASP:HB3	1:A:84:ASN:H	1.60	0.67
1:A:24:HIS:HE1	3:A:489:HOH:O	1.77	0.66
1:A:11:ARG:NH2	1:A:204:ASN:ND2	2.41	0.65
1:A:85:LYS:NZ	1:A:177:GLU:OE2	2.26	0.65
1:A:292:ASN:ND2	1:A:295:THR:H	1.94	0.65
1:A:154:ASP:OD2	1:A:196:ARG:HD3	1.97	0.65
1:A:277:ASN:HD22	1:A:279:ASP:N	1.87	0.65
1:A:145:ASN:ND2	1:A:155:ARG:H	1.94	0.65
1:A:71:LYS:CD	1:A:302:ASN:OD1	2.43	0.64
1:A:61:ARG:HD3	1:A:82:ASP:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASN:ND2	1:A:412:GLN:HB3	2.12	0.64
1:A:407:ASN:C	1:A:407:ASN:HD22	2.02	0.62
1:A:3:ALA:HB2	1:A:13:HIS:CE1	2.34	0.62
1:A:143:PRO:HD2	3:A:578:HOH:O	1.99	0.62
1:A:84:ASN:OD1	1:A:86:ASN:HB3	2.01	0.61
1:A:332:TYR:HB3	1:A:335:HIS:CD2	2.35	0.61
1:A:402:PHE:CD1	1:A:417:ARG:HB2	2.35	0.61
1:A:319:TYR:OH	1:A:335:HIS:HD2	1.83	0.61
1:A:88:ARG:HB2	3:A:662:HOH:O	2.01	0.61
1:A:11:ARG:HH22	1:A:204:ASN:HD21	1.46	0.60
1:A:144:GLY:O	1:A:146:TYR:N	2.32	0.60
1:A:258:LEU:HB2	1:A:273:GLY:HA3	1.84	0.60
1:A:42:GLN:HG3	3:A:597:HOH:O	2.02	0.59
1:A:3:ALA:HB1	1:A:13:HIS:NE2	2.18	0.59
1:A:3:ALA:CB	1:A:13:HIS:CE1	2.86	0.59
1:A:167:HIS:HD2	1:A:169:GLN:H	1.49	0.58
1:A:38:ILE:O	1:A:42:GLN:HG2	2.03	0.58
1:A:332:TYR:HB3	1:A:335:HIS:HD2	1.69	0.57
1:A:61:ARG:CD	1:A:84:ASN:HB3	2.31	0.57
1:A:182:ARG:HD2	1:A:211:ALA:HB2	1.85	0.57
1:A:116:ASN:ND2	1:A:117:HIS:HD2	1.90	0.56
1:A:325:SER:HB2	1:A:326:PRO:CD	2.36	0.56
1:A:299:PRO:CD	1:A:334:ASP:OD2	2.51	0.55
1:A:312:ASP:HA	1:A:315:ILE:HG13	1.88	0.55
1:A:292:ASN:HD21	1:A:294:ASP:HB2	1.71	0.55
1:A:292:ASN:HD22	1:A:294:ASP:H	1.54	0.55
1:A:19:ILE:HD13	1:A:328:THR:CG2	2.38	0.54
1:A:61:ARG:HB3	1:A:84:ASN:O	2.08	0.54
1:A:321:TYR:HB2	1:A:387:LEU:HD11	1.90	0.54
1:A:402:PHE:HD1	1:A:417:ARG:HB2	1.73	0.54
1:A:122:TYR:CD1	1:A:123:PRO:HD2	2.43	0.53
1:A:87:GLY:O	1:A:88:ARG:HB2	2.09	0.53
1:A:335:HIS:HE1	3:A:522:HOH:O	1.92	0.53
1:A:333:TRP:HD1	1:A:334:ASP:OD1	1.92	0.53
1:A:88:ARG:NH1	3:A:564:HOH:O	2.41	0.53
1:A:355:ALA:CB	1:A:381:GLN:HB2	2.39	0.53
1:A:404:GLU:OE1	1:A:407:ASN:HB2	2.09	0.53
1:A:167:HIS:CD2	1:A:169:GLN:HB3	2.43	0.53
1:A:191:ARG:NH1	1:A:193:ASP:HB2	2.23	0.52
1:A:11:ARG:NH1	1:A:204:ASN:ND2	2.42	0.52
1:A:114:VAL:O	1:A:114:VAL:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:HA2	3:A:562:HOH:O	2.10	0.52
1:A:43:ALA:HB2	1:A:102:LEU:HD13	1.91	0.52
1:A:323:LEU:O	1:A:352:ARG:HD2	2.10	0.52
1:A:390:ASP:O	1:A:391:LEU:C	2.48	0.51
1:A:122:TYR:CG	1:A:123:PRO:HD2	2.46	0.51
1:A:244:ASP:O	1:A:248:ARG:HG3	2.10	0.51
1:A:26:ASN:ND2	1:A:29:ARG:HH11	2.01	0.51
1:A:2:GLN:O	1:A:14:GLY:HA3	2.10	0.51
1:A:220:LEU:HD23	1:A:242:ILE:HD12	1.92	0.51
1:A:61:ARG:HD3	1:A:82:ASP:CB	2.42	0.50
1:A:29:ARG:NH2	1:A:76:GLU:OE2	2.24	0.50
1:A:366:HIS:HB2	1:A:373:VAL:HG22	1.92	0.50
1:A:143:PRO:HB2	1:A:146:TYR:CE1	2.38	0.50
1:A:195:VAL:CG1	1:A:220:LEU:HB2	2.41	0.50
1:A:279:ASP:OD1	1:A:280:PRO:HD2	2.11	0.50
1:A:81:HIS:HD2	3:A:495:HOH:O	1.94	0.50
1:A:200:PRO:HB2	1:A:248:ARG:HB2	1.94	0.49
1:A:319:TYR:O	1:A:323:LEU:HB2	2.12	0.49
1:A:320:ALA:HA	1:A:348:LEU:HD13	1.95	0.49
1:A:137:ARG:NH2	1:A:146:TYR:O	2.33	0.48
1:A:167:HIS:CD2	1:A:169:GLN:H	2.30	0.48
1:A:19:ILE:HD13	1:A:328:THR:HG22	1.95	0.48
1:A:43:ALA:CB	1:A:102:LEU:HD13	2.44	0.48
1:A:373:VAL:HA	1:A:385:VAL:O	2.13	0.48
1:A:195:VAL:HG11	1:A:220:LEU:HB2	1.96	0.47
1:A:115:PRO:HG2	1:A:198:TYR:CZ	2.49	0.46
1:A:417:ARG:CG	3:A:544:HOH:O	2.63	0.46
1:A:111:TYR:CD2	1:A:187:ALA:HB2	2.50	0.46
1:A:202:ARG:O	1:A:205:SER:HB2	2.16	0.46
1:A:325:SER:HB2	1:A:326:PRO:HD2	1.99	0.45
1:A:145:ASN:ND2	1:A:154:ASP:HB3	2.09	0.45
1:A:382:THR:O	1:A:417:ARG:HB3	2.17	0.45
1:A:292:ASN:HD22	1:A:294:ASP:N	2.13	0.45
1:A:42:GLN:CG	3:A:597:HOH:O	2.63	0.45
1:A:145:ASN:HD21	1:A:155:ARG:H	1.65	0.44
1:A:323:LEU:HA	1:A:323:LEU:HD12	1.88	0.44
1:A:60:TRP:HB3	1:A:82:ASP:O	2.18	0.44
1:A:1:ASP:OD2	1:A:108:LYS:NZ	2.51	0.44
1:A:387:LEU:O	1:A:388:ASN:C	2.56	0.44
1:A:292:ASN:HD22	1:A:292:ASN:C	2.22	0.44
1:A:292:ASN:ND2	1:A:294:ASP:N	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:HG2	1:A:198:TYR:CE2	2.53	0.43
1:A:261:ARG:NE	1:A:261:ARG:HA	2.32	0.43
1:A:344:PHE:CZ	1:A:348:LEU:HD11	2.53	0.43
1:A:194:PHE:O	1:A:194:PHE:CD2	2.72	0.43
1:A:182:ARG:HD2	1:A:211:ALA:CB	2.49	0.43
1:A:118:MET:O	1:A:161:ALA:HB1	2.20	0.42
1:A:191:ARG:HH11	1:A:193:ASP:HB2	1.85	0.42
1:A:35:TRP:CE3	1:A:38:ILE:HD12	2.54	0.42
1:A:96:ARG:HD3	1:A:96:ARG:HH11	1.66	0.42
1:A:78:TYR:O	1:A:117:HIS:HE1	2.02	0.42
1:A:66:TRP:CE3	1:A:66:TRP:O	2.73	0.42
1:A:372:LEU:HA	3:A:480:HOH:O	2.21	0.41
1:A:69:GLY:O	1:A:70:SER:C	2.58	0.41
1:A:3:ALA:HB1	1:A:13:HIS:CE1	2.55	0.41
1:A:11:ARG:NH2	1:A:204:ASN:HD21	2.14	0.41
1:A:237:SER:H	1:A:240:GLN:HE21	1.68	0.41
1:A:409:SER:O	1:A:412:GLN:CG	2.63	0.40
1:A:150:CYS:O	1:A:164:ASN:HB2	2.22	0.40
1:A:282:TRP:O	1:A:285:VAL:HG22	2.22	0.40
1:A:306:HIS:ND1	1:A:306:HIS:O	2.54	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	416/429 (97%)	386 (93%)	21 (5%)	9 (2%)	8 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	SER

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Mol	Chain	Res	Type
1	A	71	LYS
1	A	87	GLY
1	A	133	GLN
1	A	68	ASP
1	A	123	PRO
1	A	132	GLY
1	A	301	GLN
1	A	157	ILE

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	333/337 (99%)	296 (89%)	37 (11%)	8 6

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	19	ILE
1	A	55	TRP
1	A	61	ARG
1	A	68	ASP
1	A	71	LYS
1	A	79	PHE
1	A	86	ASN
1	A	95	LEU
1	A	102	LEU
1	A	109	VAL
1	A	119	ASN
1	A	125	LYS
1	A	146	TYR
1	A	157	ILE
1	A	160	ASP
1	A	162	ASP
1	A	195	VAL

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Mol	Chain	Res	Type
1	A	196	ARG
1	A	248	ARG
1	A	290	VAL
1	A	292	ASN
1	A	308	TRP
1	A	317	GLN
1	A	323	LEU
1	A	353	ARG
1	A	358	ARG
1	A	364	SER
1	A	367	SER
1	A	373	VAL
1	A	383	LEU
1	A	389	SER
1	A	397	VAL
1	A	404	GLU
1	A	407	ASN
1	A	409	SER
1	A	418	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	24	HIS
1	A	26	ASN
1	A	81	HIS
1	A	97	GLN
1	A	117	HIS
1	A	119	ASN
1	A	145	ASN
1	A	167	HIS
1	A	180	ASN
1	A	204	ASN
1	A	240	GLN
1	A	264	ASN
1	A	277	ASN
1	A	292	ASN
1	A	317	GLN
1	A	335	HIS
1	A	366	HIS
1	A	388	ASN

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Mol	Chain	Res	Type
1	A	407	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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	418/429 (97%)	0.29	15 (3%) 46 45	8, 19, 39, 62	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	SER	10.5
1	A	68	ASP	9.0
1	A	67	SER	7.2
1	A	2	GLN	6.8
1	A	1	ASP	6.0
1	A	146	TYR	5.8
1	A	69	GLY	4.6
1	A	71	LYS	4.5
1	A	3	ALA	4.3
1	A	72	SER	3.2
1	A	418	SER	3.0
1	A	66	TRP	2.9
1	A	302	ASN	2.5
1	A	87	GLY	2.1
1	A	86	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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	CA	A	455	1/1	0.78	0.17	-0.51	58,58,58,58	0
2	CA	A	454	1/1	0.98	0.03	-5.61	17,17,17,17	0

6.5 Other polymers

There are no such residues in this entry.