Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:44 AM GMT

PDB ID	:	3MYP
Title	:	Crystal structure of tagatose-1,6-bisphosphate aldolase from Staphylococcus aureus
Authors	:	Lee, S.J.; Kim, H.S.; Kim, D.J.; Yoon, H.J.; Kim, K.H.; Yoon, J.Y.; Suh, S.W.
Deposited on	:	2010-05-10
Resolution	:	2.99 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 ⓘ symbol.

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

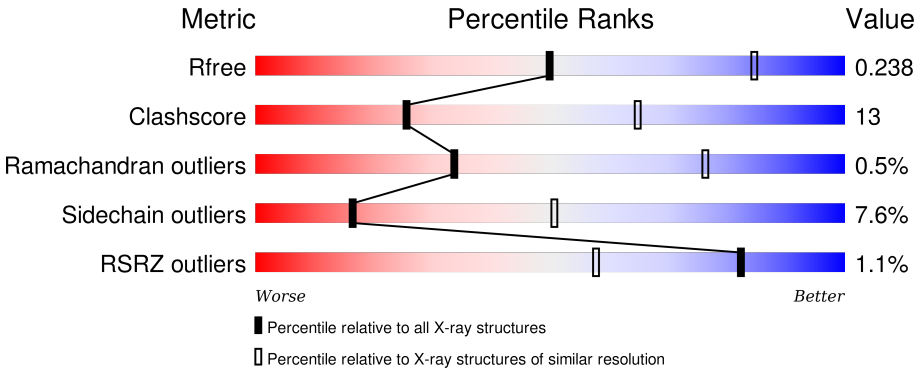
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.99 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	334	65% 28%
1	B	334	75% 20%
1	C	334	72% 21%
1	D	334	71% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10232 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 Tagatose 1,6-diphosphate aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	Se	0	0	0
			2534	1608	422	496	4	4			
1	B	321	Total	C	N	O	S	Se	0	0	0
			2534	1608	422	496	4	4			
1	C	321	Total	C	N	O	S	Se	0	0	0
			2534	1608	422	496	4	4			
1	D	321	Total	C	N	O	S	Se	0	0	0
			2534	1608	422	496	4	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	LEU	-	EXPRESSION TAG	UNP Q5HE13
A	328	GLU	-	EXPRESSION TAG	UNP Q5HE13
A	329	HIS	-	EXPRESSION TAG	UNP Q5HE13
A	330	HIS	-	EXPRESSION TAG	UNP Q5HE13
A	331	HIS	-	EXPRESSION TAG	UNP Q5HE13
A	332	HIS	-	EXPRESSION TAG	UNP Q5HE13
A	333	HIS	-	EXPRESSION TAG	UNP Q5HE13
A	334	HIS	-	EXPRESSION TAG	UNP Q5HE13
B	327	LEU	-	EXPRESSION TAG	UNP Q5HE13
B	328	GLU	-	EXPRESSION TAG	UNP Q5HE13
B	329	HIS	-	EXPRESSION TAG	UNP Q5HE13
B	330	HIS	-	EXPRESSION TAG	UNP Q5HE13
B	331	HIS	-	EXPRESSION TAG	UNP Q5HE13
B	332	HIS	-	EXPRESSION TAG	UNP Q5HE13
B	333	HIS	-	EXPRESSION TAG	UNP Q5HE13
B	334	HIS	-	EXPRESSION TAG	UNP Q5HE13
C	327	LEU	-	EXPRESSION TAG	UNP Q5HE13
C	328	GLU	-	EXPRESSION TAG	UNP Q5HE13
C	329	HIS	-	EXPRESSION TAG	UNP Q5HE13
C	330	HIS	-	EXPRESSION TAG	UNP Q5HE13
C	331	HIS	-	EXPRESSION TAG	UNP Q5HE13

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Chain	Residue	Modelled	Actual	Comment	Reference
C	332	HIS	-	EXPRESSION TAG	UNP Q5HE13
C	333	HIS	-	EXPRESSION TAG	UNP Q5HE13
C	334	HIS	-	EXPRESSION TAG	UNP Q5HE13
D	327	LEU	-	EXPRESSION TAG	UNP Q5HE13
D	328	GLU	-	EXPRESSION TAG	UNP Q5HE13
D	329	HIS	-	EXPRESSION TAG	UNP Q5HE13
D	330	HIS	-	EXPRESSION TAG	UNP Q5HE13
D	331	HIS	-	EXPRESSION TAG	UNP Q5HE13
D	332	HIS	-	EXPRESSION TAG	UNP Q5HE13
D	333	HIS	-	EXPRESSION TAG	UNP Q5HE13
D	334	HIS	-	EXPRESSION TAG	UNP Q5HE13

- Molecule 2 is water.

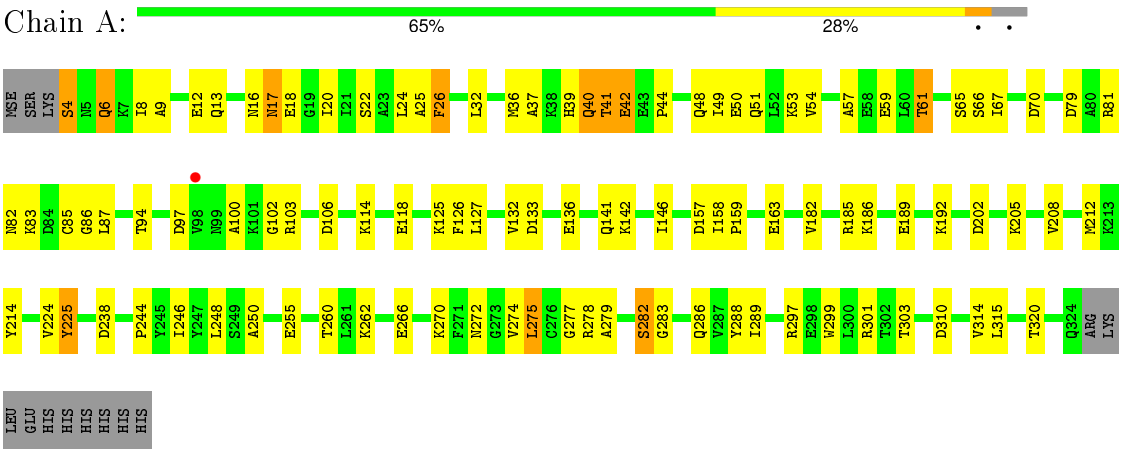
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	19	Total O 19 19	0	0
2	B	20	Total O 20 20	0	0
2	C	28	Total O 28 28	0	0
2	D	29	Total O 29 29	0	0

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.

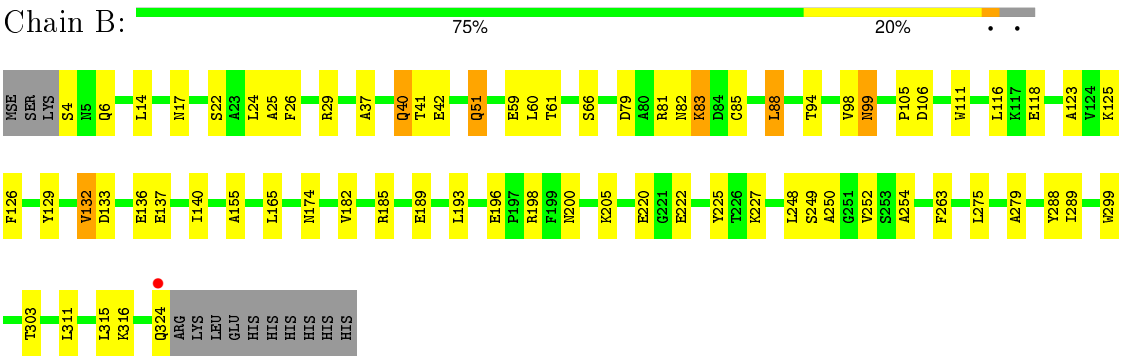
- Molecule 1: Tagatose 1,6-diphosphate aldolase

Chain A:



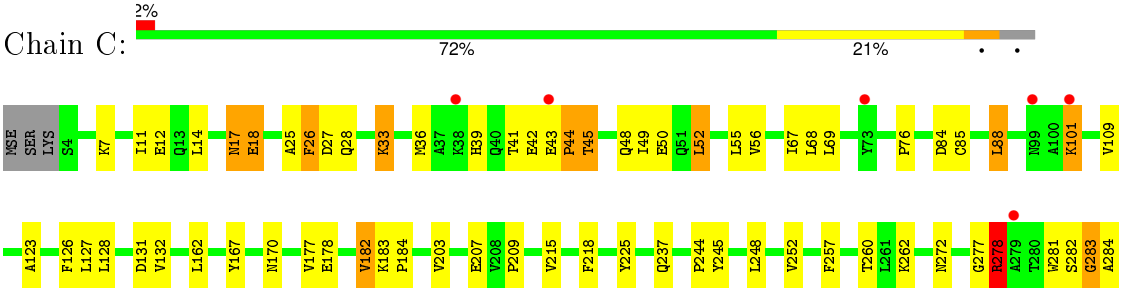
- Molecule 1: Tagatose 1,6-diphosphate aldolase

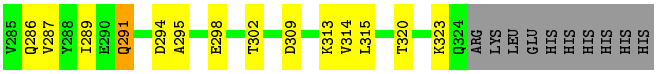
Chain B:



- Molecule 1: Tagatose 1,6-diphosphate aldolase

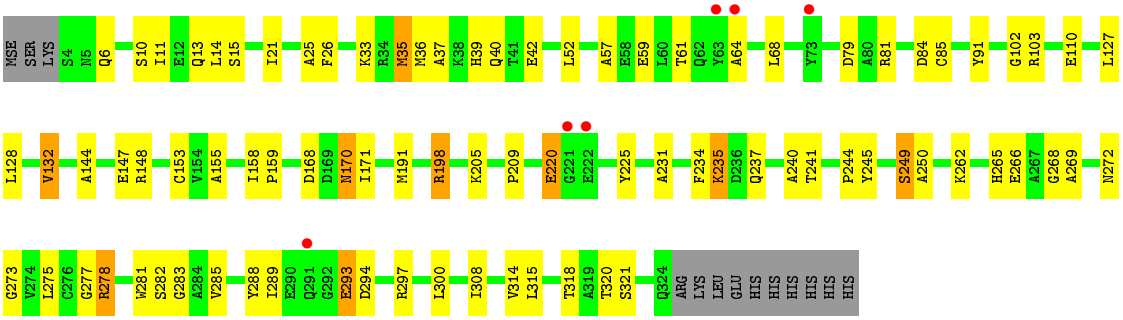
Chain C:





• Molecule 1: Tagatose 1,6-diphosphate aldolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	104.90Å 104.90Å 115.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.83 – 2.99 19.82 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.83-2.99) 99.3 (19.82-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.203 , 0.241 0.201 , 0.238	Depositor DCC
R_{free} test set	1447 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 16.3	EDS
Estimated twinning fraction	0.037 for -h,-k,l 0.186 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 28578 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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	0.53	0/2577	0.75	1/3479 (0.0%)
1	B	0.50	0/2577	0.72	0/3479
1	C	0.51	1/2577 (0.0%)	0.74	0/3479
1	D	0.51	0/2577	0.71	0/3479
All	All	0.51	1/10308 (0.0%)	0.73	1/13916 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	CYS	CB-SG	-5.33	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40	GLN	N-CA-C	5.90	126.93	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2534	0	2494	87	0
1	B	2534	0	2494	58	0
1	C	2534	0	2494	54	0
1	D	2534	0	2494	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	0	5	0
2	B	20	0	0	2	0
2	C	28	0	0	6	0
2	D	29	0	0	2	0
All	All	10232	0	9976	252	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 13.

All (252) 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:39:HIS:CE1	1:A:286:GLN:HE21	1.43	1.34
1:A:39:HIS:HE1	1:A:286:GLN:NE2	1.35	1.24
1:B:248:LEU:HD12	1:B:250:ALA:HB2	1.33	1.09
1:A:37:ALA:O	1:A:41:THR:HA	1.51	1.08
1:A:212:MSE:HE2	1:A:260:THR:HG23	1.41	1.02
1:B:40:GLN:HB3	1:B:41:THR:HA	1.41	1.00
1:C:170:ASN:ND2	2:C:352:HOH:O	1.84	0.98
1:C:278:ARG:HG2	1:C:278:ARG:HH11	1.28	0.94
1:A:255:GLU:OE2	2:A:340:HOH:O	1.89	0.90
1:C:17:ASN:ND2	1:C:17:ASN:H	1.66	0.89
1:A:25:ALA:HB2	1:A:275:LEU:CD2	2.02	0.88
1:A:25:ALA:HB2	1:A:275:LEU:HD23	1.54	0.88
1:C:50:GLU:OE1	1:C:76:PRO:HG2	1.77	0.84
1:C:45:THR:HG23	1:C:48:GLN:HB2	1.61	0.82
1:A:53:LYS:NZ	1:A:70:ASP:OD1	2.14	0.81
1:B:40:GLN:HB3	1:B:41:THR:CA	2.11	0.80
1:D:205:LYS:HE3	1:D:275:LEU:HD22	1.62	0.80
1:B:248:LEU:CD1	1:B:250:ALA:HB2	2.10	0.79
1:C:17:ASN:H	1:C:17:ASN:HD22	1.28	0.78
1:B:94:THR:HG22	2:B:346:HOH:O	1.83	0.78
1:A:26:PHE:HE1	1:A:53:LYS:HA	1.48	0.77
1:D:57:ALA:O	1:D:61:THR:OG1	2.02	0.76
1:A:40:GLN:NE2	1:A:289:ILE:HG23	2.01	0.76
1:B:137:GLU:HB2	2:B:340:HOH:O	1.85	0.75
1:C:17:ASN:O	2:C:335:HOH:O	2.04	0.74
1:A:37:ALA:O	1:A:41:THR:CA	2.34	0.74
1:B:249:SER:O	1:B:252:VAL:HG22	1.88	0.73
1:A:26:PHE:CE1	1:A:53:LYS:HA	2.22	0.73
1:D:61:THR:HG21	1:D:81:ARG:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:SER:HA	1:A:85:CYS:O	1.90	0.72
1:A:86:GLY:O	2:A:343:HOH:O	2.08	0.71
1:A:16:ASN:C	1:A:16:ASN:OD1	2.30	0.70
1:B:61:THR:HG23	1:B:85:CYS:SG	2.32	0.70
1:B:125:LYS:HD2	1:B:205:LYS:HZ3	1.54	0.70
1:C:101:LYS:HD2	1:C:101:LYS:H	1.57	0.69
1:C:88:LEU:HD12	1:C:88:LEU:N	2.08	0.69
1:C:17:ASN:ND2	1:C:17:ASN:N	2.39	0.69
1:A:87:LEU:HA	2:A:343:HOH:O	1.91	0.69
1:A:17:ASN:HD22	1:A:18:GLU:H	1.42	0.68
1:B:40:GLN:CB	1:B:41:THR:HA	2.17	0.67
1:B:14:LEU:HD11	1:B:123:ALA:HB2	1.77	0.67
1:D:205:LYS:CE	1:D:275:LEU:HD22	2.25	0.67
1:A:39:HIS:CE1	1:A:286:GLN:NE2	2.25	0.66
1:C:278:ARG:CG	1:C:278:ARG:HH11	2.07	0.66
1:A:16:ASN:OD1	1:A:18:GLU:N	2.28	0.66
1:D:39:HIS:ND1	2:D:362:HOH:O	2.28	0.66
1:A:40:GLN:HE22	1:A:48:GLN:HE22	1.44	0.66
1:A:42:GLU:O	1:A:44:PRO:HD3	1.95	0.66
1:D:59:GLU:OE2	1:D:297:ARG:NH1	2.30	0.64
1:C:257:PHE:O	1:C:260:THR:HB	1.98	0.63
1:D:25:ALA:HB2	1:D:275:LEU:CD2	2.29	0.63
1:A:205:LYS:NZ	1:A:275:LEU:HD22	2.14	0.63
1:D:191:MSE:HE2	1:D:241:THR:HG21	1.80	0.62
1:C:25:ALA:HB3	1:C:277:GLY:HA2	1.82	0.61
1:B:25:ALA:HB2	1:B:275:LEU:HD21	1.82	0.61
1:B:83:LYS:HD2	1:C:283:GLY:HA2	1.82	0.61
1:B:61:THR:HG21	1:B:81:ARG:HB2	1.81	0.60
1:B:61:THR:HG21	1:B:82:ASN:H	1.67	0.60
1:D:61:THR:HG22	1:D:85:CYS:HB2	1.84	0.60
1:C:278:ARG:HA	1:C:281:TRP:NE1	2.17	0.59
1:D:314:VAL:O	1:D:318:THR:OG1	2.15	0.59
1:A:125:LYS:HG2	1:A:126:PHE:N	2.18	0.59
1:C:278:ARG:NH1	1:C:278:ARG:HG2	2.08	0.59
1:A:246:ILE:HD12	1:A:275:LEU:HB2	1.85	0.59
1:A:278:ARG:O	1:A:282:SER:HB3	2.03	0.58
1:A:25:ALA:HB2	1:A:275:LEU:HD21	1.84	0.58
1:D:25:ALA:HB2	1:D:275:LEU:HD21	1.86	0.58
1:B:205:LYS:NZ	1:B:275:LEU:HD22	2.18	0.58
1:D:10:SER:O	1:D:13:GLN:HB2	2.02	0.58
1:D:158:ILE:HG13	1:D:159:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:GLU:CD	1:D:220:GLU:H	2.07	0.58
1:B:61:THR:HG22	1:B:82:ASN:HB3	1.85	0.57
1:A:32:LEU:HD23	1:A:49:ILE:HG23	1.86	0.57
1:A:16:ASN:OD1	1:A:17:ASN:N	2.38	0.57
1:C:207:GLU:HB3	2:C:362:HOH:O	2.04	0.57
1:D:147:GLU:CD	1:D:198:ARG:HH11	2.07	0.56
1:B:118:GLU:OE2	1:D:198:ARG:NH2	2.38	0.56
1:C:88:LEU:HD12	1:C:88:LEU:H	1.70	0.56
1:C:33:LYS:HG2	1:C:44:PRO:HG2	1.86	0.56
1:B:61:THR:CG2	1:B:82:ASN:H	2.17	0.56
1:A:59:GLU:OE1	1:A:301:ARG:NE	2.38	0.56
1:A:36:MSE:HE1	1:A:49:ILE:HA	1.88	0.56
1:B:51:GLN:HG2	1:B:288:TYR:OH	2.05	0.56
1:C:36:MSE:SE	1:C:52:LEU:HD23	2.55	0.56
1:B:88:LEU:HG	1:B:123:ALA:HB3	1.89	0.56
1:A:86:GLY:C	2:A:343:HOH:O	2.44	0.55
1:C:27:ASP:HB3	1:C:68:LEU:HG	1.87	0.55
1:D:21:ILE:O	1:D:273:GLY:HA3	2.07	0.55
1:B:311:LEU:O	1:B:315:LEU:HB2	2.06	0.55
1:D:191:MSE:HE2	1:D:241:THR:CG2	2.36	0.55
1:A:97:ASP:OD2	1:A:100:ALA:HB3	2.06	0.55
1:A:208:VAL:HG11	1:A:260:THR:HG21	1.88	0.54
1:A:244:PRO:HA	1:A:272:ASN:ND2	2.22	0.54
1:D:205:LYS:HD2	1:D:275:LEU:HD13	1.90	0.54
1:B:132:VAL:HG11	1:B:189:GLU:HB3	1.90	0.54
1:D:244:PRO:HA	1:D:272:ASN:HD22	1.73	0.54
1:D:244:PRO:HA	1:D:272:ASN:ND2	2.22	0.54
1:B:40:GLN:HG2	1:B:42:GLU:HB2	1.89	0.54
1:A:17:ASN:HD22	1:A:18:GLU:N	2.05	0.53
1:A:82:ASN:CG	1:A:83:LYS:H	2.11	0.53
1:C:39:HIS:ND1	1:C:286:GLN:HG3	2.24	0.53
1:A:4:SER:O	1:A:8:ILE:HG13	2.07	0.53
1:B:133:ASP:OD2	1:B:185:ARG:NH1	2.41	0.53
1:C:203:VAL:HG22	1:C:244:PRO:HG2	1.89	0.53
1:A:132:VAL:HG11	1:A:189:GLU:CB	2.38	0.53
1:D:237:GLN:O	1:D:240:ALA:HB3	2.09	0.53
1:B:155:ALA:HB2	1:D:155:ALA:HB2	1.91	0.53
1:A:272:ASN:HA	1:A:320:THR:O	2.08	0.53
1:A:61:THR:HG21	1:A:81:ARG:HB2	1.91	0.53
1:C:183:LYS:HB3	1:C:184:PRO:HD3	1.89	0.53
1:B:82:ASN:CG	1:B:83:LYS:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLN:HG2	1:A:288:TYR:OH	2.10	0.52
1:B:25:ALA:HB2	1:B:275:LEU:CD2	2.39	0.51
1:B:40:GLN:HG2	1:B:42:GLU:H	1.75	0.51
1:C:262:LYS:HE3	1:C:314:VAL:HG13	1.93	0.51
1:A:238:ASP:OD2	1:A:270:LYS:N	2.38	0.51
1:C:126:PHE:O	1:C:162:LEU:HD12	2.11	0.51
1:A:40:GLN:C	1:A:42:GLU:HG3	2.32	0.51
1:A:97:ASP:OD2	1:A:100:ALA:CB	2.59	0.50
1:A:159:PRO:HA	1:A:202:ASP:OD2	2.12	0.50
1:A:114:LYS:O	1:A:118:GLU:HG3	2.11	0.50
1:C:209:PRO:HD3	1:C:237:GLN:OE1	2.11	0.50
1:A:133:ASP:OD2	1:A:185:ARG:NH1	2.45	0.50
1:A:40:GLN:O	1:A:42:GLU:OE2	2.30	0.50
1:D:209:PRO:HD3	1:D:237:GLN:OE1	2.11	0.50
1:D:11:ILE:HA	1:D:14:LEU:HD12	1.94	0.50
1:B:118:GLU:CD	1:D:198:ARG:HH22	2.15	0.50
1:C:84:ASP:O	1:C:84:ASP:OD1	2.30	0.50
1:B:136:GLU:O	1:B:140:ILE:HG22	2.11	0.50
1:A:132:VAL:HG11	1:A:189:GLU:HB2	1.93	0.49
1:D:168:ASP:C	1:D:168:ASP:OD1	2.49	0.49
1:C:127:LEU:HD12	1:C:128:LEU:N	2.27	0.49
1:A:283:GLY:HA3	1:A:299:TRP:CZ2	2.47	0.49
1:A:61:THR:HG22	1:A:85:CYS:SG	2.52	0.49
1:D:153:CYS:HB3	1:D:158:ILE:O	2.12	0.49
1:A:50:GLU:O	1:A:54:VAL:HG23	2.13	0.49
1:C:36:MSE:HE1	1:C:48:GLN:HG2	1.95	0.49
1:D:262:LYS:O	1:D:266:GLU:HG3	2.13	0.49
1:A:278:ARG:HB2	1:A:278:ARG:NH1	2.27	0.49
1:B:61:THR:HG22	1:B:82:ASN:CB	2.43	0.48
1:A:49:ILE:O	1:A:53:LYS:HG3	2.13	0.48
1:D:205:LYS:NZ	1:D:275:LEU:HD22	2.29	0.48
1:D:25:ALA:HA	1:D:68:LEU:HB3	1.95	0.48
1:B:193:LEU:O	1:B:196:GLU:HG3	2.13	0.48
1:D:64:ALA:HB2	1:D:308:ILE:HD11	1.95	0.48
1:D:25:ALA:CB	1:D:275:LEU:HD21	2.43	0.48
1:B:29:ARG:HB2	1:B:94:THR:HG21	1.95	0.48
1:B:193:LEU:O	1:B:196:GLU:CG	2.62	0.48
1:C:7:LYS:NZ	2:C:336:HOH:O	2.43	0.48
1:B:14:LEU:HA	1:B:66:SER:HB3	1.96	0.47
1:D:288:TYR:HE1	1:D:293:GLU:HG2	1.78	0.47
1:B:105:PRO:HB2	1:B:126:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASN:N	1:A:17:ASN:ND2	2.60	0.47
1:C:245:TYR:H	1:C:272:ASN:ND2	2.12	0.47
1:A:142:LYS:O	1:A:146:ILE:HG12	2.14	0.47
1:B:25:ALA:CB	1:B:275:LEU:HD21	2.44	0.47
1:A:41:THR:O	1:A:41:THR:OG1	2.30	0.47
1:A:65:SER:O	1:A:85:CYS:O	2.33	0.47
1:B:254:ALA:HB2	1:B:279:ALA:HB1	1.97	0.47
1:D:102:GLY:O	1:D:103:ARG:C	2.54	0.47
1:D:144:ALA:O	1:D:148:ARG:HG3	2.14	0.47
1:A:24:LEU:O	1:A:67:ILE:HG13	2.15	0.47
1:A:297:ARG:O	1:A:301:ARG:HG3	2.15	0.46
1:D:277:GLY:O	1:D:278:ARG:C	2.52	0.46
1:A:248:LEU:HD12	1:A:250:ALA:HB2	1.98	0.46
1:A:16:ASN:ND2	1:A:20:ILE:HB	2.31	0.46
1:C:36:MSE:HE2	1:C:36:MSE:HB3	1.86	0.46
1:D:168:ASP:OD1	1:D:170:ASN:N	2.46	0.46
1:A:102:GLY:O	1:A:103:ARG:C	2.54	0.46
1:D:35:MSE:CE	1:D:282:SER:HB2	2.45	0.46
1:D:265:HIS:O	1:D:268:GLY:N	2.46	0.46
1:A:39:HIS:CE1	1:A:286:GLN:HB2	2.50	0.46
1:A:141:GLN:HG2	1:C:109:VAL:HB	1.97	0.46
1:D:231:ALA:O	1:D:235:LYS:HG3	2.16	0.46
1:A:17:ASN:H	1:A:17:ASN:ND2	2.14	0.46
1:C:67:ILE:HG12	1:C:69:LEU:HG	1.97	0.46
1:D:6:GLN:NE2	1:D:6:GLN:O	2.29	0.46
1:B:37:ALA:O	1:B:41:THR:HG23	2.16	0.45
1:B:40:GLN:HB3	1:B:42:GLU:N	2.31	0.45
1:B:25:ALA:HB2	1:B:275:LEU:CG	2.46	0.45
1:A:127:LEU:HA	1:A:163:GLU:HB3	1.99	0.45
1:D:61:THR:CG2	1:D:85:CYS:CB	2.95	0.45
1:B:99:ASN:H	1:B:99:ASN:ND2	2.14	0.45
1:C:45:THR:O	1:C:49:ILE:HG13	2.17	0.45
1:C:215:VAL:O	1:C:218:PHE:HB2	2.16	0.45
1:B:83:LYS:HG3	1:B:83:LYS:H	1.39	0.45
1:B:83:LYS:CD	1:C:283:GLY:HA2	2.47	0.45
1:A:6:GLN:HA	1:A:6:GLN:HE21	1.82	0.45
1:A:274:VAL:HG22	1:A:315:LEU:HD21	1.98	0.44
1:D:132:VAL:O	2:D:336:HOH:O	2.21	0.44
1:A:132:VAL:HG13	2:A:346:HOH:O	2.17	0.44
1:C:131:ASP:HB2	1:C:167:TYR:O	2.17	0.44
1:A:182:VAL:O	1:A:186:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:HB2	1:B:275:LEU:HG	2.00	0.44
1:B:185:ARG:O	1:B:189:GLU:HB2	2.18	0.44
1:D:281:TRP:CE3	1:D:282:SER:HA	2.52	0.44
1:C:132:VAL:O	2:C:337:HOH:O	2.21	0.44
1:A:17:ASN:N	1:A:17:ASN:HD22	2.16	0.43
1:A:22:SER:OG	1:A:65:SER:OG	2.25	0.43
1:C:14:LEU:HD11	1:C:123:ALA:HB2	2.00	0.43
1:A:225:TYR:N	1:A:225:TYR:CD2	2.87	0.43
1:C:11:ILE:HA	1:C:14:LEU:HD12	2.01	0.43
1:A:40:GLN:HE21	1:A:289:ILE:HG23	1.79	0.43
1:D:297:ARG:HA	1:D:300:LEU:HD12	2.00	0.43
1:B:82:ASN:OD1	1:B:83:LYS:HG3	2.19	0.43
1:B:205:LYS:HE2	1:B:205:LYS:HB3	1.72	0.43
1:B:59:GLU:O	1:B:60:LEU:HD23	2.18	0.43
1:C:178:GLU:O	1:C:182:VAL:HG23	2.19	0.43
1:A:262:LYS:O	1:A:266:GLU:HG3	2.19	0.42
1:C:12:GLU:HG2	1:C:323:LYS:NZ	2.34	0.42
1:A:205:LYS:HD2	1:A:275:LEU:HD13	2.01	0.42
1:B:205:LYS:HZ2	1:B:275:LEU:HD22	1.84	0.42
1:C:18:GLU:HG2	2:C:343:HOH:O	2.19	0.42
1:B:29:ARG:CZ	1:B:94:THR:HB	2.49	0.42
1:B:299:TRP:CE2	1:B:303:THR:HB	2.54	0.42
1:B:111:TRP:CE3	1:B:116:LEU:HD23	2.53	0.42
1:A:136:GLU:OE1	1:A:136:GLU:HA	2.19	0.42
1:A:189:GLU:OE2	1:A:192:LYS:HE3	2.20	0.42
1:A:41:THR:N	1:A:42:GLU:HG3	2.34	0.42
1:D:35:MSE:HE1	1:D:282:SER:HB2	2.01	0.42
1:D:249:SER:O	1:D:250:ALA:HB3	2.20	0.42
1:C:287:VAL:HA	1:C:291:GLN:HB2	2.02	0.42
1:C:26:PHE:CE1	1:C:56:VAL:HB	2.55	0.42
1:B:129:TYR:HA	1:B:165:LEU:O	2.19	0.42
1:B:227:LYS:HG2	1:B:263:PHE:HE1	1.84	0.42
1:C:252:VAL:HG23	1:C:257:PHE:HB2	2.01	0.42
1:D:282:SER:O	1:D:285:VAL:HG23	2.20	0.42
1:C:282:SER:O	1:C:284:ALA:N	2.52	0.42
1:A:277:GLY:O	1:A:279:ALA:N	2.53	0.42
1:A:205:LYS:HZ2	1:A:275:LEU:HD22	1.85	0.42
1:A:310:ASP:O	1:A:314:VAL:HG23	2.19	0.42
1:D:36:MSE:HE3	1:D:52:LEU:HD22	2.01	0.42
1:A:42:GLU:H	1:A:42:GLU:HG3	0.94	0.41
1:C:295:ALA:O	1:C:298:GLU:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:TYR:H	1:D:272:ASN:HD22	1.67	0.41
1:D:234:PHE:HB3	1:D:269:ALA:HB2	2.01	0.41
1:D:127:LEU:HD12	1:D:128:LEU:N	2.36	0.41
1:B:22:SER:HB3	1:B:315:LEU:CD2	2.50	0.41
1:C:28:GLN:CD	1:C:28:GLN:H	2.24	0.41
1:D:320:THR:O	1:D:321:SER:C	2.58	0.41
1:D:61:THR:HG23	1:D:85:CYS:SG	2.60	0.41
1:A:214:TYR:HB3	1:A:224:VAL:HG23	2.02	0.41
1:B:324:GLN:HG3	1:B:324:GLN:O	2.21	0.41
1:C:14:LEU:HD22	1:C:88:LEU:HD11	2.03	0.41
1:D:170:ASN:C	1:D:171:ILE:HG13	2.41	0.40
1:D:6:GLN:HE21	1:D:6:GLN:C	2.15	0.40
1:D:61:THR:CG2	1:D:85:CYS:HB2	2.51	0.40
1:A:59:GLU:OE2	1:A:301:ARG:NH2	2.54	0.40
1:C:39:HIS:CE1	1:C:286:GLN:HB2	2.57	0.40
1:D:37:ALA:O	1:D:40:GLN:O	2.40	0.40
1:A:9:ALA:O	1:A:12:GLU:HB2	2.22	0.40
1:C:309:ASP:O	1:C:313:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	319/334 (96%)	288 (90%)	30 (9%)	1 (0%)	46 84
1	B	319/334 (96%)	291 (91%)	28 (9%)	0	100 100
1	C	319/334 (96%)	296 (93%)	19 (6%)	4 (1%)	15 53
1	D	319/334 (96%)	299 (94%)	18 (6%)	2 (1%)	30 72
All	All	1276/1336 (96%)	1174 (92%)	95 (7%)	7 (0%)	34 76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	283	GLY
1	A	57	ALA
1	C	44	PRO
1	C	283	GLY
1	C	278	ARG
1	D	278	ARG
1	C	289	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	268/276 (97%)	251 (94%)	17 (6%)	22	60
1	B	268/276 (97%)	245 (91%)	23 (9%)	13	44
1	C	268/276 (97%)	246 (92%)	22 (8%)	14	46
1	D	268/276 (97%)	248 (92%)	20 (8%)	17	51
All	All	1072/1104 (97%)	990 (92%)	82 (8%)	16	51

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	GLN
1	A	13	GLN
1	A	17	ASN
1	A	26	PHE
1	A	41	THR
1	A	42	GLU
1	A	61	THR
1	A	79	ASP
1	A	94	THR
1	A	106	ASP
1	A	157	ASP
1	A	158	ILE
1	A	225	TYR
1	A	275	LEU

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Mol	Chain	Res	Type
1	A	282	SER
1	A	303	THR
1	B	4	SER
1	B	6	GLN
1	B	17	ASN
1	B	24	LEU
1	B	26	PHE
1	B	40	GLN
1	B	51	GLN
1	B	79	ASP
1	B	83	LYS
1	B	88	LEU
1	B	98	VAL
1	B	99	ASN
1	B	106	ASP
1	B	132	VAL
1	B	174	ASN
1	B	182	VAL
1	B	198	ARG
1	B	200	ASN
1	B	220	GLU
1	B	222	GLU
1	B	225	TYR
1	B	289	ILE
1	B	316	LYS
1	C	17	ASN
1	C	18	GLU
1	C	26	PHE
1	C	33	LYS
1	C	41	THR
1	C	42	GLU
1	C	43	GLU
1	C	45	THR
1	C	52	LEU
1	C	55	LEU
1	C	88	LEU
1	C	101	LYS
1	C	177	VAL
1	C	182	VAL
1	C	225	TYR
1	C	248	LEU
1	C	278	ARG

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Mol	Chain	Res	Type
1	C	291	GLN
1	C	294	ASP
1	C	302	THR
1	C	315	LEU
1	C	320	THR
1	D	15	SER
1	D	26	PHE
1	D	33	LYS
1	D	35	MSE
1	D	42	GLU
1	D	79	ASP
1	D	84	ASP
1	D	91	TYR
1	D	110	GLU
1	D	132	VAL
1	D	170	ASN
1	D	198	ARG
1	D	220	GLU
1	D	225	TYR
1	D	235	LYS
1	D	249	SER
1	D	289	ILE
1	D	293	GLU
1	D	294	ASP
1	D	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	13	GLN
1	A	17	ASN
1	A	39	HIS
1	A	48	GLN
1	A	82	ASN
1	A	242	HIS
1	A	272	ASN
1	A	286	GLN
1	A	312	ASN
1	B	6	GLN
1	B	99	ASN
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	272	ASN
1	B	312	ASN
1	B	324	GLN
1	C	17	ASN
1	C	62	GLN
1	C	272	ASN
1	C	312	ASN
1	C	324	GLN
1	D	6	GLN
1	D	170	ASN
1	D	272	ASN
1	D	286	GLN

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	317/334 (94%)	-0.04	1 (0%)	94	84	36, 54, 77, 83	0
1	B	317/334 (94%)	-0.02	1 (0%)	94	84	35, 57, 71, 76	0
1	C	317/334 (94%)	0.11	6 (1%)	70	41	36, 59, 81, 102	0
1	D	317/334 (94%)	0.10	6 (1%)	70	41	40, 56, 84, 91	0
All	All	1268/1336 (94%)	0.04	14 (1%)	82	58	35, 56, 79, 102	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	VAL	3.4
1	D	222	GLU	3.3
1	C	99	ASN	3.2
1	C	101	LYS	2.7
1	C	73	TYR	2.5
1	B	324	GLN	2.4
1	C	279	ALA	2.4
1	D	64	ALA	2.4
1	D	221	GLY	2.3
1	C	38	LYS	2.2
1	D	63	TYR	2.2
1	C	43	GLU	2.2
1	D	291	GLN	2.2
1	D	73	TYR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.