Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:16 AM GMT

PDB ID	:	3LG0
Title	:	Structure of Plasmodium falciparum ornithine delta-aminotransferase
Authors	:	Fritz-Wolf, K.; Jortzik, E.; Stumpf, M.; Becker, K.
Deposited on	:	2010-01-19
Resolution	:	2.30 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:

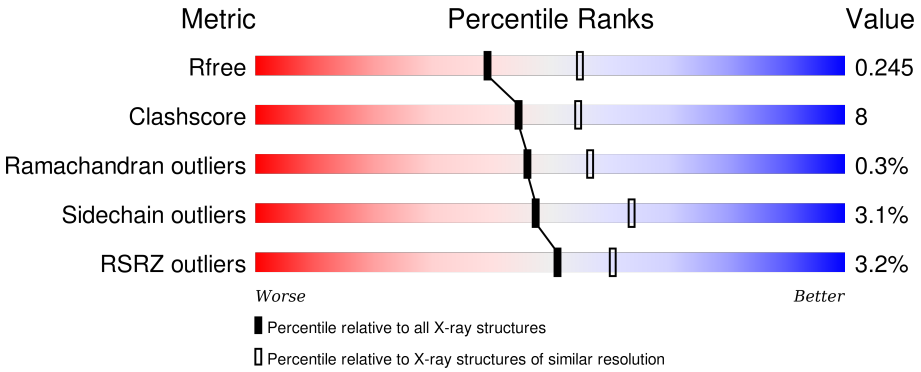
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	422	2% 74% 16% • 9%
1	B	422	4% 74% 17% • 9%
1	C	422	3% 73% 18% • 9%
1	D	422	3% 76% 14% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12470 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 Ornithine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3016	1931	502	564	19			
1	B	385	Total	C	N	O	S	0	0	0
			3016	1931	502	564	19			
1	C	385	Total	C	N	O	S	0	0	0
			3011	1925	502	565	19			
1	D	387	Total	C	N	O	S	0	0	0
			3027	1938	504	566	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	LEU	-	EXPRESSION TAG	UNP Q07805
A	416	GLN	-	EXPRESSION TAG	UNP Q07805
A	417	HIS	-	EXPRESSION TAG	UNP Q07805
A	418	HIS	-	EXPRESSION TAG	UNP Q07805
A	419	HIS	-	EXPRESSION TAG	UNP Q07805
A	420	HIS	-	EXPRESSION TAG	UNP Q07805
A	421	HIS	-	EXPRESSION TAG	UNP Q07805
A	422	HIS	-	EXPRESSION TAG	UNP Q07805
B	415	LEU	-	EXPRESSION TAG	UNP Q07805
B	416	GLN	-	EXPRESSION TAG	UNP Q07805
B	417	HIS	-	EXPRESSION TAG	UNP Q07805
B	418	HIS	-	EXPRESSION TAG	UNP Q07805
B	419	HIS	-	EXPRESSION TAG	UNP Q07805
B	420	HIS	-	EXPRESSION TAG	UNP Q07805
B	421	HIS	-	EXPRESSION TAG	UNP Q07805
B	422	HIS	-	EXPRESSION TAG	UNP Q07805
C	415	LEU	-	EXPRESSION TAG	UNP Q07805
C	416	GLN	-	EXPRESSION TAG	UNP Q07805
C	417	HIS	-	EXPRESSION TAG	UNP Q07805
C	418	HIS	-	EXPRESSION TAG	UNP Q07805
C	419	HIS	-	EXPRESSION TAG	UNP Q07805

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Chain	Residue	Modelled	Actual	Comment	Reference
C	420	HIS	-	EXPRESSION TAG	UNP Q07805
C	421	HIS	-	EXPRESSION TAG	UNP Q07805
C	422	HIS	-	EXPRESSION TAG	UNP Q07805
D	415	LEU	-	EXPRESSION TAG	UNP Q07805
D	416	GLN	-	EXPRESSION TAG	UNP Q07805
D	417	HIS	-	EXPRESSION TAG	UNP Q07805
D	418	HIS	-	EXPRESSION TAG	UNP Q07805
D	419	HIS	-	EXPRESSION TAG	UNP Q07805
D	420	HIS	-	EXPRESSION TAG	UNP Q07805
D	421	HIS	-	EXPRESSION TAG	UNP Q07805
D	422	HIS	-	EXPRESSION TAG	UNP Q07805

- Molecule 2 is water.

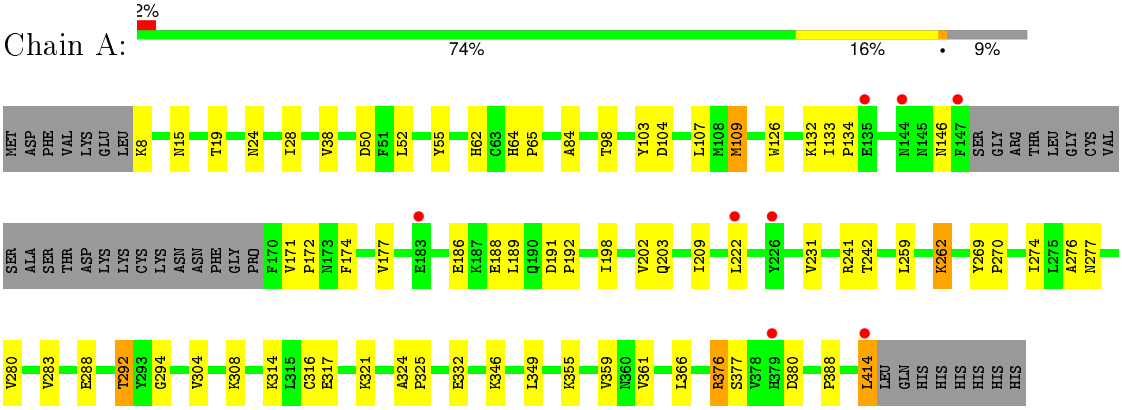
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	103	Total O 103 103	0	0
2	B	91	Total O 91 91	0	0
2	C	102	Total O 102 102	0	0
2	D	104	Total O 104 104	0	0

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.

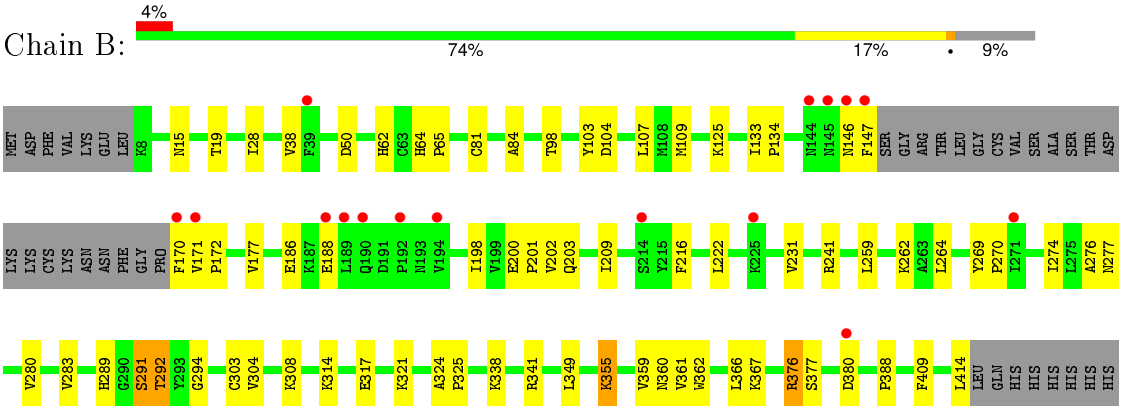
- Molecule 1: Ornithine aminotransferase

Chain A:



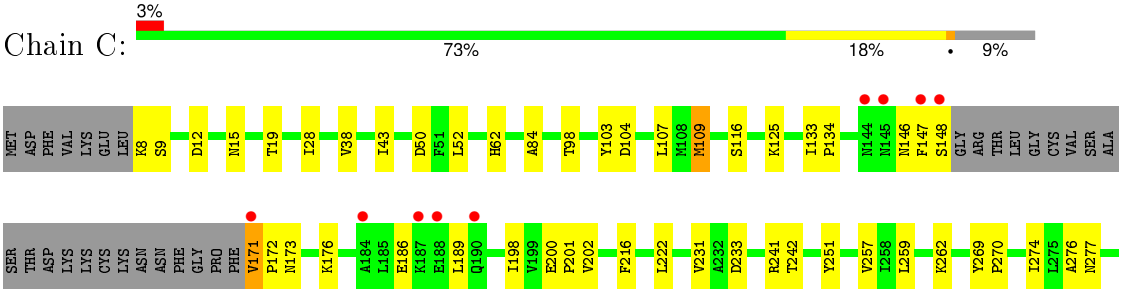
- Molecule 1: Ornithine aminotransferase

Chain B:

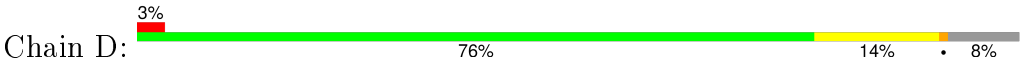


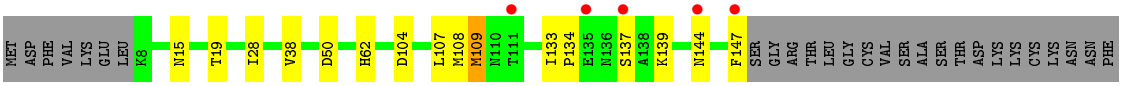
- Molecule 1: Ornithine aminotransferase

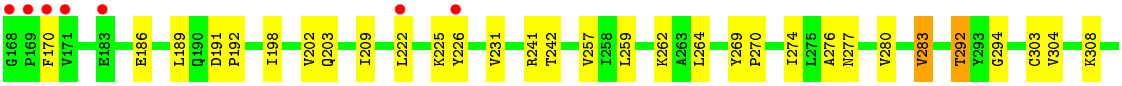
Chain C:

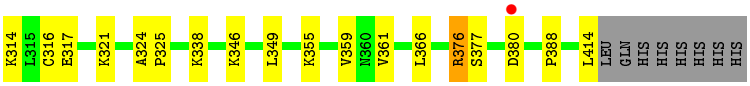


- Molecule 1: Ornithine aminotransferase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.53Å 106.93Å 147.14Å 90.00° 91.28° 90.00°	Depositor
Resolution (Å)	43.38 – 2.30 43.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (43.38-2.30) 95.4 (43.37-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.203 , 0.250 0.199 , 0.245	Depositor DCC
R_{free} test set	3973 reflections (6.00%)	DCC
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.2	EDS
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 66243 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12470	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.89 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.8726e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.39	0/3076	0.54	0/4164
1	B	0.39	0/3076	0.54	1/4164 (0.0%)
1	C	0.38	0/3070	0.53	0/4156
1	D	0.39	0/3088	0.54	0/4181
All	All	0.39	0/12310	0.54	1/16665 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	CYS	N-CA-C	-5.01	97.47	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	3016	0	3034	49	0
1	B	3016	0	3034	48	0
1	C	3011	0	3030	59	0
1	D	3027	0	3044	45	0
2	A	103	0	0	3	0
2	B	91	0	0	2	0
2	C	102	0	0	9	0
2	D	104	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12470	0	12142	191	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 8.

All (191) 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:C:292:THR:HG22	1:C:294:GLY:H	1.34	0.93
1:A:38:VAL:HG23	1:A:388:PRO:HD2	1.61	0.82
1:C:171:VAL:HG23	1:C:172:PRO:HD2	1.62	0.82
1:C:276:ALA:HB1	1:C:280:VAL:CG2	2.12	0.80
1:D:38:VAL:HG23	1:D:388:PRO:HD2	1.65	0.79
1:C:38:VAL:HG23	1:C:388:PRO:HD2	1.62	0.79
1:B:38:VAL:HG23	1:B:388:PRO:HD2	1.65	0.78
1:A:292:THR:HG22	1:A:294:GLY:H	1.47	0.77
1:A:276:ALA:HB1	1:A:280:VAL:CG2	2.13	0.77
1:B:276:ALA:HB1	1:B:280:VAL:CG2	2.15	0.76
1:D:276:ALA:HB1	1:D:280:VAL:CG2	2.16	0.75
1:B:147:PHE:HB3	2:B:462:HOH:O	1.85	0.75
1:D:292:THR:HG22	1:D:294:GLY:H	1.51	0.75
1:A:332:GLU:HG2	2:A:525:HOH:O	1.87	0.73
1:D:50:ASP:OD2	1:D:62:HIS:HE1	1.72	0.73
1:B:50:ASP:OD2	1:B:62:HIS:HE1	1.72	0.73
1:A:50:ASP:OD2	1:A:62:HIS:HE1	1.72	0.71
1:C:50:ASP:OD2	1:C:62:HIS:HE1	1.74	0.70
1:C:292:THR:CG2	1:C:294:GLY:H	2.04	0.68
1:C:376:ARG:HH11	1:C:376:ARG:HG2	1.59	0.68
1:B:171:VAL:HG23	1:B:172:PRO:HD2	1.75	0.68
1:D:147:PHE:HB3	2:D:485:HOH:O	1.95	0.67
1:C:15:ASN:O	1:C:19:THR:HG23	1.95	0.67
1:B:276:ALA:HB1	1:B:280:VAL:HG21	1.78	0.66
1:C:381:LYS:HE2	2:C:523:HOH:O	1.96	0.65
1:C:109:MET:SD	2:C:513:HOH:O	2.54	0.65
1:C:276:ALA:HB1	1:C:280:VAL:HG21	1.78	0.65
1:A:109:MET:HE1	2:A:471:HOH:O	1.95	0.65
1:A:276:ALA:HB1	1:A:280:VAL:HG21	1.80	0.64
1:C:146:ASN:ND2	1:C:200:GLU:OE2	2.31	0.63
1:B:15:ASN:O	1:B:19:THR:HG23	1.99	0.62
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.64	0.62
1:A:15:ASN:O	1:A:19:THR:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ARG:HG2	1:D:376:ARG:HH11	1.63	0.62
1:B:376:ARG:HG2	1:B:376:ARG:HH11	1.64	0.61
1:D:276:ALA:HB1	1:D:280:VAL:HG21	1.82	0.61
1:D:15:ASN:O	1:D:19:THR:HG23	2.01	0.61
1:D:316:CYS:SG	2:D:520:HOH:O	2.56	0.61
1:C:304:VAL:HG12	1:C:308:LYS:HE2	1.84	0.60
1:C:148:SER:HB3	1:C:176:LYS:NZ	2.17	0.60
1:A:146:ASN:HB3	1:A:203:GLN:NE2	2.17	0.59
1:C:109:MET:HG3	2:C:513:HOH:O	2.01	0.59
1:B:146:ASN:ND2	1:B:200:GLU:OE2	2.31	0.59
1:A:304:VAL:HG12	1:A:308:LYS:HE2	1.84	0.58
1:B:304:VAL:HG12	1:B:308:LYS:HE2	1.86	0.58
1:D:304:VAL:HG12	1:D:308:LYS:HE2	1.86	0.58
1:A:276:ALA:HB1	1:A:280:VAL:HG23	1.87	0.57
1:C:84:ALA:HB1	1:D:376:ARG:HD3	1.87	0.56
1:D:280:VAL:O	1:D:283:VAL:HB	2.06	0.56
1:C:276:ALA:HB1	1:C:280:VAL:HG23	1.87	0.56
1:D:276:ALA:HB1	1:D:280:VAL:HG23	1.88	0.55
1:D:139:LYS:NZ	2:D:528:HOH:O	2.35	0.55
1:D:314:LYS:HA	1:D:317:GLU:OE1	2.08	0.54
1:B:292:THR:HG22	1:B:294:GLY:H	1.73	0.54
1:C:62:HIS:HD2	2:D:505:HOH:O	1.90	0.54
1:B:314:LYS:HA	1:B:317:GLU:OE1	2.08	0.54
1:A:280:VAL:O	1:A:283:VAL:HB	2.08	0.54
1:C:251:TYR:HA	2:C:456:HOH:O	2.08	0.53
1:A:314:LYS:HA	1:A:317:GLU:OE1	2.08	0.53
1:B:170:PHE:CD2	1:B:171:VAL:N	2.77	0.52
1:C:172:PRO:O	1:C:173:ASN:HB2	2.09	0.52
1:C:171:VAL:HG23	1:C:172:PRO:CD	2.37	0.52
1:D:241:ARG:HG3	1:D:349:LEU:HB2	1.92	0.51
1:A:414:LEU:HD12	1:A:414:LEU:H	1.73	0.51
1:C:361:VAL:HG12	1:C:377:SER:HB3	1.93	0.51
1:A:292:THR:CG2	1:A:294:GLY:H	2.21	0.51
1:A:55:TYR:CD2	1:B:291:SER:HB3	2.46	0.51
1:C:292:THR:HG22	1:C:294:GLY:N	2.15	0.50
1:C:314:LYS:HA	1:C:317:GLU:OE1	2.10	0.50
1:D:226:TYR:HE2	2:D:522:HOH:O	1.93	0.50
1:A:241:ARG:HG3	1:A:349:LEU:HB2	1.94	0.50
1:A:38:VAL:HA	1:A:388:PRO:HG2	1.93	0.50
1:A:316:CYS:SG	2:A:438:HOH:O	2.60	0.50
1:D:137:SER:HB2	2:D:528:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:SER:HG	1:C:147:PHE:HZ	1.60	0.49
1:C:269:TYR:CZ	1:D:270:PRO:HD3	2.48	0.49
1:A:24:ASN:O	1:B:289:HIS:CE1	2.66	0.49
1:A:262:LYS:NZ	1:B:291:SER:HB2	2.27	0.49
1:D:361:VAL:HG12	1:D:377:SER:HB3	1.95	0.49
1:B:361:VAL:HG12	1:B:377:SER:HB3	1.94	0.49
1:D:259:LEU:HD22	1:D:274:ILE:HG12	1.94	0.49
1:B:276:ALA:HB1	1:B:280:VAL:HG23	1.93	0.48
1:A:84:ALA:HB1	1:B:376:ARG:HD3	1.94	0.48
1:D:38:VAL:HA	1:D:388:PRO:HG2	1.96	0.48
1:B:314:LYS:HE2	2:B:498:HOH:O	2.11	0.48
1:A:28:ILE:HD12	1:A:366:LEU:HD23	1.96	0.48
1:C:50:ASP:OD2	1:C:62:HIS:CE1	2.63	0.48
1:A:304:VAL:CG1	1:A:308:LYS:HE2	2.44	0.48
1:C:147:PHE:HB3	2:C:501:HOH:O	2.12	0.48
1:B:104:ASP:HB2	1:B:277:ASN:HA	1.95	0.47
1:C:109:MET:CG	2:C:513:HOH:O	2.58	0.47
1:D:324:ALA:HB3	1:D:325:PRO:HD3	1.96	0.47
1:A:126:TRP:HA	1:A:283:VAL:HG21	1.95	0.47
1:B:125:LYS:HG2	1:B:283:VAL:HG13	1.97	0.47
1:A:361:VAL:HG12	1:A:377:SER:HB3	1.96	0.47
1:C:241:ARG:HG3	1:C:349:LEU:HB2	1.96	0.47
1:B:38:VAL:HA	1:B:388:PRO:HG2	1.96	0.47
1:C:38:VAL:HA	1:C:388:PRO:HG2	1.96	0.46
1:D:28:ILE:HD12	1:D:366:LEU:HD23	1.96	0.46
1:D:304:VAL:CG1	1:D:308:LYS:HE2	2.45	0.46
1:A:198:ILE:HG12	1:A:231:VAL:HB	1.97	0.46
1:B:241:ARG:HG3	1:B:349:LEU:HB2	1.96	0.46
1:C:270:PRO:HD3	1:D:269:TYR:CZ	2.50	0.46
1:C:8:LYS:HA	1:C:12:ASP:OD2	2.16	0.46
1:C:285:LYS:O	1:C:287:GLY:N	2.49	0.46
1:A:50:ASP:OD2	1:A:62:HIS:CE1	2.62	0.46
1:C:147:PHE:CE1	1:C:233:ASP:OD2	2.69	0.46
1:C:98:THR:HB	1:C:103:TYR:O	2.16	0.46
1:C:9:SER:HA	1:C:43:ILE:HG21	1.97	0.46
1:C:125:LYS:HG2	1:C:283:VAL:HG13	1.98	0.45
1:C:304:VAL:CG1	1:C:308:LYS:HE2	2.46	0.45
1:B:186:GLU:HB2	1:B:222:LEU:HD13	1.99	0.45
1:A:104:ASP:HB2	1:A:277:ASN:HA	1.98	0.45
1:C:198:ILE:HG12	1:C:231:VAL:HB	1.99	0.45
1:A:376:ARG:HD3	1:B:84:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:THR:HB	1:C:346:LYS:HG2	1.99	0.45
1:C:259:LEU:HD22	1:C:274:ILE:HG12	1.99	0.45
1:C:104:ASP:HB2	1:C:277:ASN:HA	1.98	0.45
1:A:186:GLU:HB2	1:A:222:LEU:HD13	1.99	0.44
1:A:98:THR:HB	1:A:103:TYR:O	2.17	0.44
1:D:292:THR:CG2	1:D:294:GLY:H	2.27	0.44
1:A:324:ALA:HB3	1:A:325:PRO:HD3	1.99	0.44
1:B:367:LYS:HE2	1:B:409:PHE:CD1	2.52	0.44
1:C:324:ALA:HB3	1:C:325:PRO:HD3	1.99	0.44
1:A:270:PRO:HD3	1:B:269:TYR:CZ	2.53	0.44
1:B:259:LEU:HD22	1:B:274:ILE:HG12	2.00	0.44
1:A:203:GLN:HB2	1:A:209:ILE:HB	2.00	0.44
1:C:292:THR:HG22	1:C:293:TYR:N	2.32	0.44
1:B:50:ASP:OD2	1:B:62:HIS:CE1	2.60	0.44
1:C:133:ILE:HG23	1:C:134:PRO:HD2	2.01	0.43
1:D:50:ASP:OD2	1:D:62:HIS:CE1	2.61	0.43
1:A:189:LEU:HD12	1:A:222:LEU:HB3	2.00	0.43
1:B:338:LYS:HB2	1:B:338:LYS:HE2	1.82	0.43
1:B:341:ARG:CZ	1:B:355:LYS:HD2	2.49	0.43
1:D:317:GLU:O	1:D:321:LYS:HG3	2.19	0.43
1:D:198:ILE:HG12	1:D:231:VAL:HB	2.00	0.43
1:A:242:THR:HB	1:A:346:LYS:HG2	1.99	0.43
1:D:133:ILE:HG23	1:D:134:PRO:HD2	2.00	0.43
1:D:242:THR:HB	1:D:346:LYS:HG2	2.00	0.43
1:C:381:LYS:HE3	2:C:427:HOH:O	2.18	0.42
1:B:304:VAL:CG1	1:B:308:LYS:HE2	2.48	0.42
1:D:191:ASP:HA	1:D:192:PRO:HD2	1.87	0.42
1:D:231:VAL:HG22	1:D:257:VAL:HB	2.01	0.42
1:A:317:GLU:O	1:A:321:LYS:HG3	2.19	0.42
1:D:189:LEU:HD12	1:D:222:LEU:HB3	2.01	0.42
1:C:231:VAL:HG22	1:C:257:VAL:HB	2.01	0.42
1:B:203:GLN:HB2	1:B:209:ILE:HB	2.01	0.42
1:B:324:ALA:HB3	1:B:325:PRO:HD3	2.01	0.42
1:B:201:PRO:HA	1:B:216:PHE:CZ	2.54	0.42
1:A:177:VAL:CG1	1:A:188:GLU:HG3	2.50	0.42
1:A:259:LEU:HD22	1:A:274:ILE:HG12	2.01	0.42
1:C:52:LEU:HA	1:C:52:LEU:HD12	1.89	0.42
1:B:198:ILE:HG12	1:B:231:VAL:HB	2.01	0.42
1:C:189:LEU:HD12	1:C:222:LEU:HB3	2.02	0.42
1:B:264:LEU:HD22	1:B:303:CYS:SG	2.59	0.42
1:B:177:VAL:CG1	1:B:188:GLU:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:524:HOH:O	1:D:62:HIS:HD2	2.03	0.42
1:A:52:LEU:HA	1:A:52:LEU:HD12	1.88	0.42
1:C:201:PRO:HA	1:C:216:PHE:CZ	2.55	0.42
1:D:203:GLN:HB2	1:D:209:ILE:HB	2.02	0.42
1:B:317:GLU:O	1:B:321:LYS:HG3	2.20	0.41
1:B:28:ILE:HD12	1:B:366:LEU:HD23	2.02	0.41
1:A:171:VAL:HA	1:A:172:PRO:HD3	1.98	0.41
1:A:269:TYR:CZ	1:B:270:PRO:HD3	2.55	0.41
1:B:376:ARG:HG2	1:B:376:ARG:NH1	2.35	0.41
1:C:148:SER:HB3	1:C:176:LYS:HZ1	1.86	0.41
1:A:171:VAL:HG13	1:A:174:PHE:HB2	2.03	0.41
1:D:104:ASP:HB2	1:D:277:ASN:HA	2.03	0.41
1:C:376:ARG:HH11	1:C:376:ARG:CG	2.30	0.41
1:C:341:ARG:CZ	1:C:355:LYS:HD2	2.50	0.41
1:D:225:LYS:HD3	2:D:522:HOH:O	2.20	0.41
1:B:98:THR:HB	1:B:103:TYR:O	2.20	0.41
1:B:292:THR:CG2	1:B:294:GLY:H	2.33	0.41
1:A:64:HIS:HA	1:A:65:PRO:HD3	1.87	0.41
1:D:108:MET:C	1:D:109:MET:HG2	2.41	0.41
1:A:133:ILE:HG23	1:A:134:PRO:HD2	2.03	0.41
1:B:133:ILE:HG23	1:B:134:PRO:HD2	2.03	0.41
1:D:170:PHE:CD2	1:D:170:PHE:C	2.94	0.41
1:A:191:ASP:HA	1:A:192:PRO:HD2	1.89	0.41
1:B:64:HIS:HA	1:B:65:PRO:HD3	1.85	0.41
1:D:186:GLU:HB2	1:D:222:LEU:HD13	2.03	0.40
1:C:186:GLU:HB2	1:C:222:LEU:HD13	2.02	0.40
1:C:28:ILE:HD12	1:C:366:LEU:HD23	2.02	0.40
1:C:360:ASN:OD1	1:C:362:TRP:HB3	2.20	0.40
1:D:264:LEU:HD22	1:D:303:CYS:SG	2.61	0.40
1:A:132:LYS:HA	1:A:132:LYS:HD3	1.92	0.40
1:C:356:ASN:ND2	2:C:523:HOH:O	2.48	0.40
1:C:317:GLU:O	1:C:321:LYS:HG3	2.21	0.40
1:D:376:ARG:CG	1:D:376:ARG:HH11	2.33	0.40
1:B:360:ASN:OD1	1:B:362:TRP:HB3	2.21	0.40
1:D:338:LYS:HB2	1:D:338:LYS:HE2	1.83	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	381/422 (90%)	370 (97%)	10 (3%)	1 (0%)	46	57
1	B	381/422 (90%)	368 (97%)	12 (3%)	1 (0%)	46	57
1	C	381/422 (90%)	364 (96%)	15 (4%)	2 (0%)	34	41
1	D	383/422 (91%)	369 (96%)	13 (3%)	1 (0%)	46	57
All	All	1526/1688 (90%)	1471 (96%)	50 (3%)	5 (0%)	46	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	LYS
1	B	262	LYS
1	C	262	LYS
1	D	262	LYS
1	C	286	PRO

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	335/368 (91%)	324 (97%)	11 (3%)	45	61
1	B	335/368 (91%)	325 (97%)	10 (3%)	48	65
1	C	335/368 (91%)	326 (97%)	9 (3%)	52	70
1	D	336/368 (91%)	325 (97%)	11 (3%)	45	61
All	All	1341/1472 (91%)	1300 (97%)	41 (3%)	47	64

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	107	LEU
1	A	109	MET
1	A	202	VAL
1	A	288	GLU
1	A	292	THR
1	A	355	LYS
1	A	359	VAL
1	A	376	ARG
1	A	380	ASP
1	A	414	LEU
1	B	107	LEU
1	B	109	MET
1	B	202	VAL
1	B	291	SER
1	B	292	THR
1	B	355	LYS
1	B	359	VAL
1	B	376	ARG
1	B	380	ASP
1	B	414	LEU
1	C	107	LEU
1	C	109	MET
1	C	171	VAL
1	C	202	VAL
1	C	292	THR
1	C	355	LYS
1	C	359	VAL
1	C	376	ARG
1	C	380	ASP
1	D	107	LEU
1	D	109	MET
1	D	144	ASN
1	D	202	VAL
1	D	283	VAL
1	D	292	THR
1	D	355	LYS
1	D	359	VAL
1	D	376	ARG
1	D	380	ASP
1	D	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	203	GLN
1	A	268	HIS
1	A	289	HIS
1	A	333	GLN
1	A	371	ASN
1	B	62	HIS
1	B	203	GLN
1	B	289	HIS
1	B	333	GLN
1	B	371	ASN
1	C	62	HIS
1	C	333	GLN
1	C	371	ASN
1	D	62	HIS
1	D	203	GLN
1	D	268	HIS
1	D	333	GLN
1	D	371	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

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	385/422 (91%)	0.17	8 (2%) 67 74	20, 39, 66, 92	0
1	B	385/422 (91%)	0.33	16 (4%) 40 49	20, 40, 69, 123	0
1	C	385/422 (91%)	0.15	13 (3%) 49 58	20, 39, 67, 105	0
1	D	387/422 (91%)	0.18	13 (3%) 49 58	21, 38, 67, 102	0
All	All	1542/1688 (91%)	0.21	50 (3%) 51 60	20, 39, 68, 123	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	PHE	14.5
1	B	171	VAL	11.4
1	D	168	GLY	8.2
1	C	171	VAL	6.4
1	C	288	GLU	5.1
1	A	183	GLU	3.9
1	C	190	GLN	3.7
1	C	380	ASP	3.4
1	D	380	ASP	3.4
1	D	135	GLU	3.3
1	A	222	LEU	3.1
1	C	184	ALA	3.1
1	D	183	GLU	3.1
1	D	169	PRO	3.1
1	B	188	GLU	3.1
1	A	147	PHE	3.1
1	B	145	ASN	3.0
1	B	192	PRO	2.9
1	B	189	LEU	2.8
1	C	144	ASN	2.8
1	B	225	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	190	GLN	2.7
1	D	222	LEU	2.7
1	C	145	ASN	2.7
1	C	357	ASP	2.7
1	D	226	TYR	2.6
1	A	135	GLU	2.6
1	B	144	ASN	2.6
1	D	147	PHE	2.5
1	C	188	GLU	2.5
1	C	359	VAL	2.5
1	A	379	HIS	2.5
1	B	214	SER	2.5
1	B	380	ASP	2.5
1	B	146	ASN	2.5
1	D	170	PHE	2.5
1	A	414	LEU	2.4
1	C	187	LYS	2.4
1	B	147	PHE	2.4
1	C	147	PHE	2.4
1	A	226	TYR	2.3
1	B	39	PHE	2.3
1	D	137	SER	2.3
1	B	194	VAL	2.2
1	B	271	ILE	2.2
1	D	171	VAL	2.2
1	A	144	ASN	2.1
1	D	111	THR	2.0
1	C	148	SER	2.0
1	D	144	ASN	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.