Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 PM GMT

PDB ID	:	4MY5
Title	:	Crystal structure of the aromatic amino acid aminotransferase from Streptococcus mutants
Authors	:	Cong, X.; Li, X.; Ge, J.; Feng, Y.; Feng, X.; Li, S.
Deposited on	:	2013-09-27
Resolution	:	2.19 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:

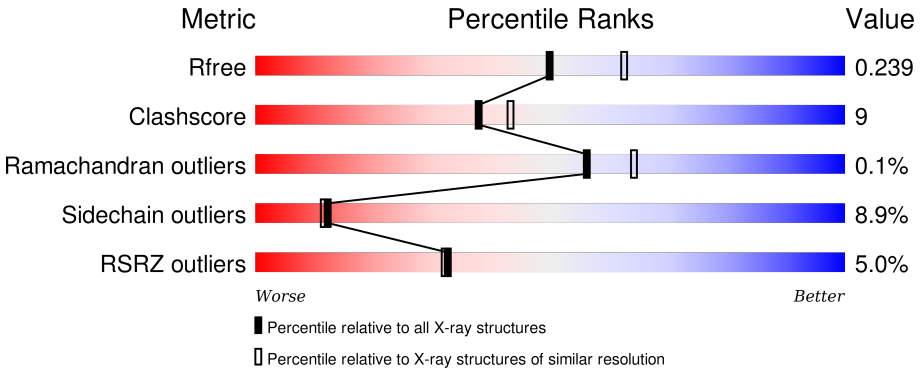
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.19 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	3774 (2.20-2.20)
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	393	2% 77% 18%
1	B	393	5% 77% 17%
1	C	393	2% 76% 19% 5%
1	D	393	11% 71% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12983 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 Putative amino acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3032	1961	487	573	11			
1	D	377	Total	C	N	O	S	0	0	0
			2901	1878	470	544	9			
1	B	382	Total	C	N	O	S	0	0	0
			2951	1910	474	558	9			
1	C	388	Total	C	N	O	S	0	0	0
			3019	1951	488	570	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q8DWM1
A	0	PRO	-	EXPRESSION TAG	UNP Q8DWM1
D	-1	GLY	-	EXPRESSION TAG	UNP Q8DWM1
D	0	PRO	-	EXPRESSION TAG	UNP Q8DWM1
B	-1	GLY	-	EXPRESSION TAG	UNP Q8DWM1
B	0	PRO	-	EXPRESSION TAG	UNP Q8DWM1
C	-1	GLY	-	EXPRESSION TAG	UNP Q8DWM1
C	0	PRO	-	EXPRESSION TAG	UNP Q8DWM1

- Molecule 2 is water.

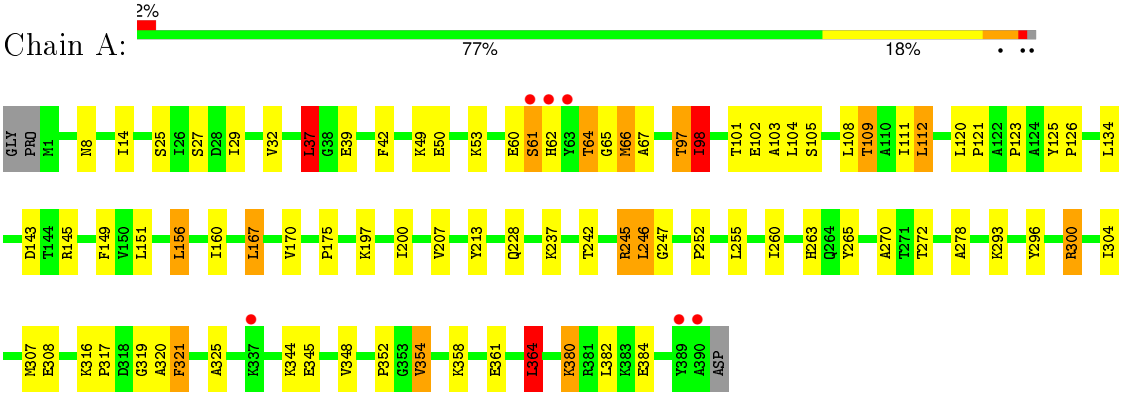
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	341	Total	O	0	0
			341	341		
2	D	183	Total	O	0	0
			183	183		
2	B	267	Total	O	0	0
			267	267		
2	C	289	Total	O	0	0
			289	289		

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.

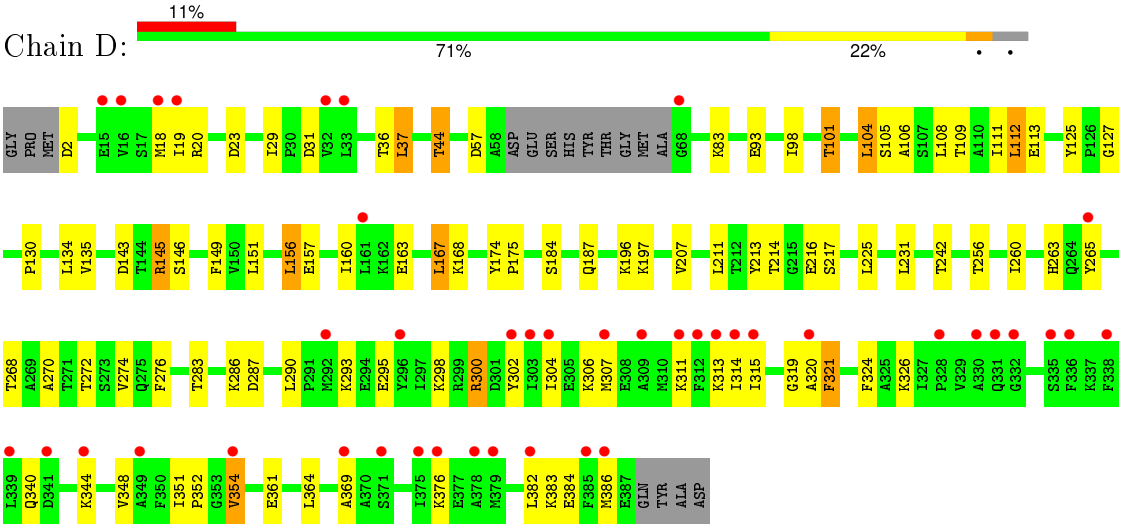
- Molecule 1: Putative amino acid aminotransferase

Chain A:



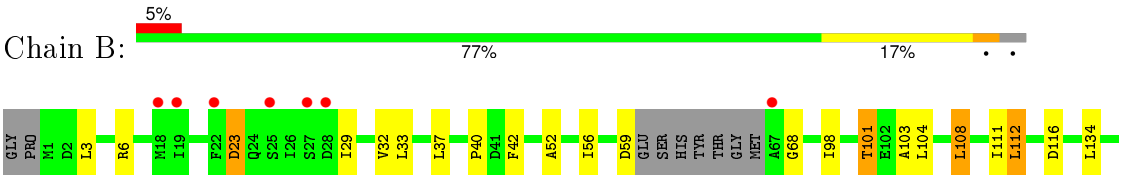
- Molecule 1: Putative amino acid aminotransferase

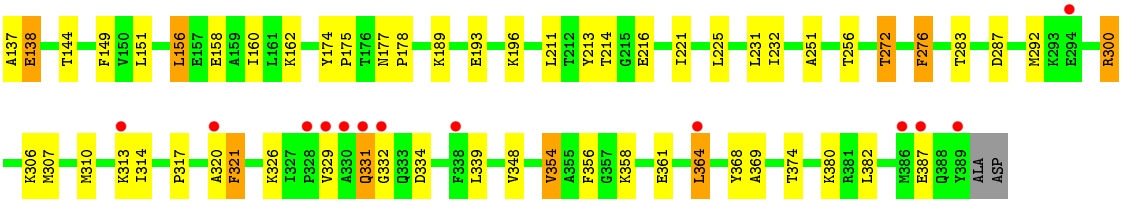
Chain D:



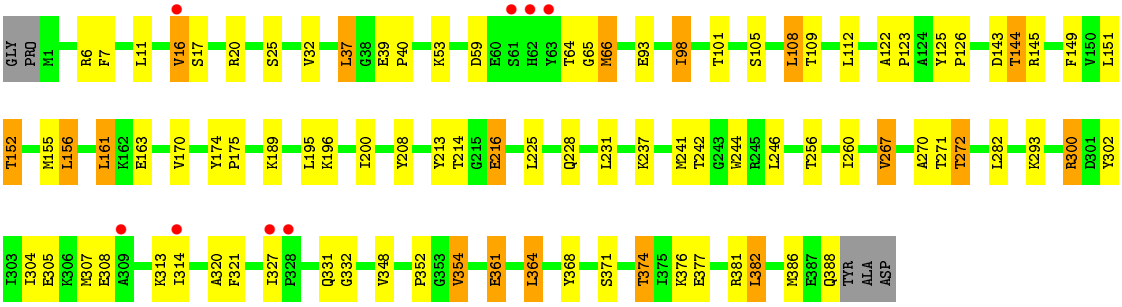
- Molecule 1: Putative amino acid aminotransferase

Chain B:





- Molecule 1: Putative amino acid 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	104.75Å 64.26Å 125.60Å 90.00° 106.77° 90.00°	Depositor
Resolution (Å)	52.49 – 2.19 54.11 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.4 (52.49-2.19) 93.5 (54.11-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.191 , 0.239 0.190 , 0.239	Depositor DCC
R_{free} test set	3860 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 77005 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12983	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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 54.57 % 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 3.5853e-05.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	0.44	0/3094	0.64	2/4193 (0.0%)
1	B	0.41	0/3010	0.60	1/4083 (0.0%)
1	C	0.42	0/3080	0.63	1/4173 (0.0%)
1	D	0.36	0/2959	0.56	0/4015
All	All	0.41	0/12143	0.61	4/16464 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	364	LEU	CA-CB-CG	7.28	132.04	115.30
1	C	364	LEU	CA-CB-CG	6.86	131.09	115.30
1	B	364	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	37	LEU	CA-CB-CG	5.35	127.60	115.30

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	3032	0	3061	56	0
1	B	2951	0	2969	54	0
1	C	3019	0	3062	57	0
1	D	2901	0	2907	59	0
2	A	341	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	267	0	0	17	0
2	C	289	0	0	11	0
2	D	183	0	0	13	0
All	All	12983	0	11999	219	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 9.

All (219) 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:68:GLY:O	2:B:520:HOH:O	1.86	0.94
1:D:143:ASP:OD2	2:D:537:HOH:O	1.87	0.91
1:C:152:THR:HG22	1:C:155:MET:H	1.38	0.87
1:C:308:GLU:O	2:C:497:HOH:O	1.95	0.84
1:A:8:ASN:ND2	2:A:475:HOH:O	2.12	0.81
1:C:144:THR:HG23	1:C:149:PHE:HA	1.62	0.80
1:A:308:GLU:OE1	2:A:590:HOH:O	2.01	0.79
1:D:57:ASP:OD2	1:C:53:LYS:NZ	2.14	0.79
1:A:213:TYR:OH	1:A:320:ALA:HB2	1.82	0.76
1:B:213:TYR:OH	1:B:320:ALA:HB2	1.85	0.76
1:B:283:THR:O	2:B:475:HOH:O	2.02	0.76
1:A:151:LEU:HD21	1:A:156:LEU:HG	1.68	0.75
1:C:161:LEU:O	2:C:480:HOH:O	2.04	0.75
1:D:157:GLU:OE2	1:D:197:LYS:NZ	2.20	0.74
1:B:287:ASP:OD2	2:B:604:HOH:O	2.06	0.74
1:D:213:TYR:OH	1:D:320:ALA:HB2	1.89	0.73
1:B:380:LYS:NZ	2:B:609:HOH:O	2.21	0.73
1:C:213:TYR:OH	1:C:320:ALA:HB2	1.89	0.72
1:A:358:LYS:O	2:A:604:HOH:O	2.07	0.71
1:A:270:ALA:O	2:A:480:HOH:O	2.06	0.71
1:D:2:ASP:O	2:D:576:HOH:O	2.08	0.71
1:A:60:GLU:OE1	2:A:564:HOH:O	2.09	0.70
1:B:292:MET:SD	2:B:498:HOH:O	2.50	0.69
1:A:111:ILE:HG13	1:A:112:LEU:HD13	1.76	0.68
1:C:282:LEU:O	2:C:429:HOH:O	2.13	0.67
1:D:113:GLU:OE1	2:D:481:HOH:O	2.12	0.66
1:C:241:MET:O	2:C:673:HOH:O	2.14	0.66
1:A:361:GLU:O	2:A:494:HOH:O	2.13	0.66
1:C:270:ALA:O	2:C:514:HOH:O	2.12	0.66
1:A:97:THR:HG21	1:A:103:ALA:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:MET:O	2:A:669:HOH:O	2.13	0.66
1:C:354:VAL:HG13	1:C:361:GLU:HG2	1.77	0.65
1:D:217:SER:HB3	2:D:540:HOH:O	1.97	0.64
1:B:329:VAL:HG23	1:B:331:GLN:HB2	1.80	0.64
1:B:193:GLU:HA	1:B:196:LYS:HE3	1.79	0.63
1:A:66:MET:HB2	1:A:260:ILE:HD11	1.81	0.63
1:B:354:VAL:HG13	1:B:361:GLU:HG2	1.82	0.62
1:D:29:ILE:HD11	1:D:344:LYS:HG3	1.82	0.62
1:A:61:SER:OG	1:A:62:HIS:N	2.33	0.62
1:D:263:HIS:NE2	2:D:511:HOH:O	2.31	0.62
1:C:216:GLU:OE1	2:C:625:HOH:O	2.16	0.61
1:A:97:THR:HG22	1:A:247:GLY:HA3	1.82	0.61
1:D:344:LYS:NZ	2:D:442:HOH:O	2.34	0.60
1:D:20:ARG:HH22	1:C:65:GLY:HA3	1.67	0.60
1:C:214:THR:HG21	2:C:537:HOH:O	2.00	0.60
1:B:272:THR:O	1:B:276:PHE:HB3	2.01	0.60
1:D:211:LEU:HB3	1:D:320:ALA:HB3	1.84	0.60
1:D:105:SER:O	1:D:109:THR:HG23	2.02	0.59
1:D:302:TYR:CZ	1:D:376:LYS:HG2	2.38	0.59
1:A:380:LYS:NZ	2:A:509:HOH:O	2.28	0.59
1:D:23:ASP:OD2	2:D:528:HOH:O	2.17	0.59
1:B:313:LYS:HB2	1:B:326:LYS:HB3	1.85	0.58
1:D:214:THR:HG22	1:D:216:GLU:H	1.67	0.58
1:A:304:ILE:HD11	1:A:317:PRO:HG2	1.85	0.58
1:B:162:LYS:HE3	2:B:642:HOH:O	2.03	0.58
1:D:37:LEU:HD12	1:D:37:LEU:H	1.68	0.58
1:D:160:ILE:HG23	1:D:167:LEU:HD12	1.86	0.58
1:B:331:GLN:N	1:B:332:GLY:HA3	2.18	0.58
2:A:705:HOH:O	1:B:101:THR:HG21	2.03	0.58
1:D:384:GLU:OE1	2:D:523:HOH:O	2.18	0.57
1:D:151:LEU:HD21	1:D:156:LEU:HG	1.87	0.56
1:C:32:VAL:HG12	2:C:438:HOH:O	2.05	0.56
1:D:304:ILE:HG12	1:D:314:ILE:HG21	1.87	0.56
1:C:151:LEU:HD21	1:C:156:LEU:HG	1.87	0.56
1:B:104:LEU:O	1:B:108:LEU:HB2	2.06	0.56
1:D:36:THR:HA	2:D:412:HOH:O	2.06	0.56
1:A:345:GLU:OE1	2:A:639:HOH:O	2.18	0.56
1:D:174:TYR:HA	1:D:175:PRO:C	2.26	0.55
1:A:102:GLU:OE2	2:A:547:HOH:O	2.18	0.55
1:C:105:SER:O	1:C:109:THR:HG23	2.07	0.55
1:D:295:GLU:HA	1:D:298:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:SER:OG	1:C:374:THR:HG23	2.07	0.54
2:D:457:HOH:O	1:C:271:THR:HA	2.08	0.54
1:B:307:MET:HB2	1:B:314:ILE:HD11	1.89	0.54
1:A:228:GLN:HB2	1:B:3:LEU:HD11	1.90	0.53
1:A:67:ALA:HA	2:A:669:HOH:O	2.08	0.53
1:B:300:ARG:HB2	1:B:368:TYR:CZ	2.43	0.53
1:D:196:LYS:HD2	2:D:472:HOH:O	2.07	0.53
1:B:151:LEU:HD21	1:B:156:LEU:HG	1.90	0.52
1:C:144:THR:CG2	1:C:149:PHE:HA	2.37	0.52
1:A:265:TYR:O	2:A:507:HOH:O	2.19	0.52
1:D:19:ILE:HG23	1:D:351:ILE:HD12	1.92	0.52
1:C:302:TYR:CZ	1:C:376:LYS:HG2	2.44	0.52
1:D:130:PRO:HD3	2:D:520:HOH:O	2.09	0.52
1:B:326:LYS:HD2	2:B:473:HOH:O	2.10	0.51
1:A:384:GLU:OE1	2:A:557:HOH:O	2.19	0.51
1:C:16:VAL:HG23	1:C:20:ARG:HD2	1.91	0.51
1:D:101:THR:HG23	2:C:411:HOH:O	2.10	0.51
1:D:168:LYS:HE2	1:C:6:ARG:NH2	2.25	0.51
1:A:352:PRO:HB2	1:A:354:VAL:HG23	1.93	0.51
1:C:170:VAL:HG23	1:C:200:ILE:HD12	1.93	0.51
1:C:64:THR:N	1:C:65:GLY:HA2	2.25	0.51
1:A:49:LYS:O	1:A:53:LYS:HG3	2.10	0.51
1:A:37:LEU:HD13	1:A:39:GLU:O	2.11	0.50
1:B:358:LYS:HG2	2:B:438:HOH:O	2.10	0.50
1:B:211:LEU:HB3	1:B:320:ALA:HB3	1.93	0.50
1:A:325:ALA:HB3	1:A:364:LEU:HD22	1.94	0.50
1:D:111:ILE:HG13	1:D:112:LEU:HD13	1.93	0.50
1:D:382:LEU:O	1:D:386:MET:HG2	2.12	0.50
1:C:189:LYS:NZ	2:C:636:HOH:O	2.21	0.50
1:D:352:PRO:HB2	1:D:354:VAL:HG23	1.94	0.49
1:C:213:TYR:HE1	1:C:293:LYS:HG3	1.77	0.49
1:C:123:PRO:HD3	1:C:149:PHE:CD1	2.48	0.49
1:B:320:ALA:HB1	1:B:321:PHE:HB3	1.93	0.49
1:B:189:LYS:NZ	2:B:665:HOH:O	2.45	0.49
1:A:245:ARG:NH1	2:A:470:HOH:O	2.45	0.49
1:D:354:VAL:HG13	1:D:361:GLU:HG2	1.94	0.49
1:C:98:ILE:HD11	1:C:267:VAL:HG22	1.95	0.48
1:C:66:MET:HB2	1:C:260:ILE:HD11	1.95	0.48
1:D:300:ARG:HD3	1:D:304:ILE:HD12	1.94	0.48
1:D:98:ILE:HG21	1:C:98:ILE:HD12	1.95	0.48
1:B:144:THR:OG1	1:B:149:PHE:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ALA:HB1	1:D:321:PHE:HB3	1.95	0.48
1:B:29:ILE:O	1:B:32:VAL:HG23	2.14	0.47
1:A:98:ILE:HD12	1:B:98:ILE:HG21	1.95	0.47
1:A:207:VAL:HG22	1:A:237:LYS:HG2	1.97	0.47
1:B:40:PRO:HB3	1:B:369:ALA:HB1	1.97	0.47
1:A:62:HIS:ND1	2:A:561:HOH:O	2.29	0.47
1:A:160:ILE:HG23	1:A:167:LEU:HD12	1.96	0.47
1:C:382:LEU:O	1:C:386:MET:HG2	2.14	0.47
1:D:44:THR:HG23	1:C:59:ASP:OD1	2.14	0.47
1:A:125:TYR:CD1	1:A:126:PRO:HD2	2.50	0.47
1:C:174:TYR:HA	1:C:175:PRO:C	2.35	0.46
1:B:103:ALA:HB1	1:B:232:ILE:HD12	1.97	0.46
1:D:125:TYR:CE2	1:D:127:GLY:HA3	2.50	0.46
1:C:196:LYS:HA	1:C:228:GLN:OE1	2.15	0.46
1:C:213:TYR:CE1	1:C:293:LYS:HG3	2.51	0.46
1:A:109:THR:HG22	2:B:578:HOH:O	2.15	0.46
1:B:214:THR:OG1	1:B:216:GLU:O	2.33	0.46
1:C:7:PHE:HB3	1:C:11:LEU:HD12	1.97	0.46
1:D:83:LYS:NZ	1:D:287:ASP:OD1	2.46	0.46
1:C:313:LYS:HE3	1:C:313:LYS:HB2	1.77	0.45
1:C:37:LEU:HD13	1:C:39:GLU:O	2.17	0.45
1:D:307:MET:HB2	1:D:314:ILE:HD11	1.97	0.45
1:A:64:THR:OG1	1:A:65:GLY:N	2.49	0.45
1:C:40:PRO:HD2	1:C:242:THR:HG21	1.98	0.45
1:D:149:PHE:HD2	1:D:315:ILE:HG12	1.82	0.45
1:C:108:LEU:HD12	1:C:108:LEU:HA	1.83	0.45
1:D:175:PRO:HB3	1:D:319:GLY:HA3	1.97	0.45
1:A:98:ILE:H	1:A:98:ILE:HG12	1.60	0.45
1:D:217:SER:CB	2:D:540:HOH:O	2.62	0.44
1:B:306:LYS:O	1:B:310:MET:HG3	2.18	0.44
1:D:313:LYS:HE3	1:D:326:LYS:HD3	1.99	0.44
1:C:307:MET:HB3	1:C:314:ILE:HD11	2.00	0.44
1:A:42:PHE:HE2	1:A:296:TYR:CZ	2.36	0.44
1:B:6:ARG:NH2	2:B:461:HOH:O	2.50	0.44
1:B:251:ALA:HB3	1:B:256:THR:HG22	2.00	0.44
1:C:122:ALA:O	1:C:144:THR:HG21	2.18	0.44
1:A:66:MET:HG3	1:A:66:MET:H	1.53	0.44
1:D:145:ARG:HG3	1:D:149:PHE:CE1	2.51	0.44
1:D:104:LEU:HA	1:D:104:LEU:HD12	1.86	0.44
1:A:246:LEU:HG	1:A:278:ALA:HB2	2.00	0.44
1:A:358:LYS:HE2	1:A:358:LYS:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLU:OE1	2:B:664:HOH:O	2.21	0.44
1:B:160:ILE:O	2:B:654:HOH:O	2.21	0.44
1:C:143:ASP:OD2	1:C:145:ARG:NH2	2.38	0.43
1:C:300:ARG:HD3	1:C:304:ILE:HD12	2.00	0.43
1:D:211:LEU:HD13	1:D:320:ALA:HB3	2.00	0.43
1:D:93:GLU:HA	1:D:256:THR:HG21	2.00	0.43
1:D:306:LYS:HD2	1:D:383:LYS:NZ	2.33	0.43
1:C:125:TYR:CD1	1:C:126:PRO:HD2	2.53	0.43
1:C:327:ILE:HB	1:C:332:GLY:HA3	1.99	0.43
1:D:37:LEU:HD13	1:D:369:ALA:HB3	2.00	0.43
1:D:270:ALA:HB1	1:D:274:VAL:HB	1.99	0.43
1:A:213:TYR:CE1	1:A:293:LYS:HG3	2.54	0.42
1:B:52:ALA:O	1:B:56:ILE:HG12	2.18	0.42
1:B:339:LEU:HA	1:B:339:LEU:HD23	1.83	0.42
1:A:120:LEU:HA	1:A:121:PRO:HD3	1.89	0.42
1:B:33:LEU:HD13	1:B:374:THR:HG23	2.01	0.42
1:A:380:LYS:NZ	2:A:609:HOH:O	2.43	0.42
1:D:109:THR:HG22	1:D:135:VAL:HG11	2.01	0.42
1:C:331:GLN:OE1	1:C:331:GLN:N	2.52	0.42
1:D:290:LEU:O	1:D:293:LYS:HB3	2.18	0.42
1:A:213:TYR:HE1	1:A:293:LYS:HG3	1.84	0.42
1:C:244:TRP:CD1	1:C:244:TRP:N	2.88	0.42
1:A:170:VAL:HG23	1:A:200:ILE:HD12	2.00	0.42
1:C:208:TYR:CZ	1:C:237:LYS:HE2	2.55	0.42
1:B:211:LEU:CB	1:B:320:ALA:HB3	2.49	0.42
1:B:174:TYR:HA	1:B:175:PRO:C	2.39	0.42
1:D:106:ALA:HB2	1:D:265:TYR:HB2	2.00	0.42
1:B:138:GLU:HB2	2:B:531:HOH:O	2.20	0.42
1:B:300:ARG:NH2	2:B:457:HOH:O	2.34	0.42
1:B:177:ASN:HA	1:B:178:PRO:HA	1.89	0.42
1:A:307:MET:HE3	1:A:307:MET:HB3	1.97	0.42
1:B:40:PRO:HG2	1:B:42:PHE:CE2	2.54	0.42
1:A:320:ALA:HB1	1:A:321:PHE:HB3	2.02	0.42
1:A:123:PRO:HD3	1:A:149:PHE:CD1	2.54	0.42
1:B:332:GLY:H	1:B:334:ASP:H	1.68	0.41
1:A:316:LYS:HA	1:A:317:PRO:HD3	1.81	0.41
1:C:300:ARG:HB2	1:C:368:TYR:CZ	2.55	0.41
1:B:329:VAL:CG2	1:B:331:GLN:HB2	2.48	0.41
1:A:105:SER:O	1:A:109:THR:HG23	2.19	0.41
1:C:66:MET:H	1:C:66:MET:HG2	1.62	0.41
1:B:178:PRO:HG3	1:B:356:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASP:O	1:B:137:ALA:HB1	2.20	0.41
1:C:352:PRO:HB2	1:C:354:VAL:HG23	2.01	0.41
1:B:158:GLU:OE2	2:B:656:HOH:O	2.21	0.41
1:A:213:TYR:CZ	1:A:320:ALA:HB2	2.56	0.41
1:C:377:GLU:O	1:C:381:ARG:HG3	2.20	0.41
1:D:184:SER:OG	1:D:187:GLN:HG3	2.20	0.41
1:D:213:TYR:CZ	1:D:320:ALA:HB2	2.56	0.41
1:C:272:THR:HG22	2:C:514:HOH:O	2.20	0.41
1:D:214:THR:HB	1:D:216:GLU:O	2.21	0.41
1:B:300:ARG:HB2	1:B:368:TYR:CE2	2.56	0.41
1:B:111:ILE:HG13	1:B:112:LEU:HD13	2.03	0.41
1:A:175:PRO:HB3	1:A:319:GLY:HA3	2.02	0.41
1:A:39:GLU:HB3	1:A:242:THR:HG21	2.03	0.40
1:C:195:LEU:HB2	1:C:225:LEU:HD11	2.02	0.40
1:B:211:LEU:HD13	1:B:320:ALA:HB3	2.04	0.40
1:D:31:ASP:N	1:D:31:ASP:OD1	2.54	0.40
1:B:40:PRO:HD3	1:B:321:PHE:CZ	2.56	0.40
1:C:196:LYS:HE2	1:C:196:LYS:HB3	1.89	0.40
1:C:93:GLU:HA	1:C:256:THR:HG21	2.03	0.40
1:A:29:ILE:HD11	1:A:344:LYS:HD2	2.04	0.40
1:A:300:ARG:NH2	2:A:430:HOH:O	2.44	0.40
1:B:23:ASP:OD1	2:B:660:HOH:O	2.22	0.40
1:D:283:THR:O	1:D:286:LYS:HB2	2.22	0.40
1:A:143:ASP:OD2	1:A:145:ARG:NH2	2.43	0.40
1:A:252:PRO:HG2	1:A:255:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	388/393 (99%)	378 (97%)	9 (2%)	1 (0%)	46 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	378/393 (96%)	362 (96%)	15 (4%)	1 (0%)	46 50
1	C	386/393 (98%)	369 (96%)	17 (4%)	0	100 100
1	D	373/393 (95%)	350 (94%)	23 (6%)	0	100 100
All	All	1525/1572 (97%)	1459 (96%)	64 (4%)	2 (0%)	56 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	B	317	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	318/327 (97%)	287 (90%)	31 (10%)	10 9
1	B	308/327 (94%)	286 (93%)	22 (7%)	18 19
1	C	319/327 (98%)	290 (91%)	29 (9%)	12 11
1	D	299/327 (91%)	270 (90%)	29 (10%)	10 9
All	All	1244/1308 (95%)	1133 (91%)	111 (9%)	12 11

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	25	SER
1	A	27	SER
1	A	32	VAL
1	A	37	LEU
1	A	50	GLU
1	A	61	SER
1	A	64	THR
1	A	66	MET

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Mol	Chain	Res	Type
1	A	97	THR
1	A	98	ILE
1	A	101	THR
1	A	104	LEU
1	A	108	LEU
1	A	109	THR
1	A	112	LEU
1	A	134	LEU
1	A	156	LEU
1	A	167	LEU
1	A	197	LYS
1	A	245	ARG
1	A	246	LEU
1	A	263	HIS
1	A	272	THR
1	A	300	ARG
1	A	321	PHE
1	A	348	VAL
1	A	354	VAL
1	A	364	LEU
1	A	380	LYS
1	A	382	LEU
1	D	18	MET
1	D	37	LEU
1	D	44	THR
1	D	101	THR
1	D	104	LEU
1	D	108	LEU
1	D	112	LEU
1	D	134	LEU
1	D	145	ARG
1	D	146	SER
1	D	156	LEU
1	D	163	GLU
1	D	167	LEU
1	D	207	VAL
1	D	225	LEU
1	D	231	LEU
1	D	242	THR
1	D	260	ILE
1	D	268	THR
1	D	272	THR

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Mol	Chain	Res	Type
1	D	276	PHE
1	D	300	ARG
1	D	311	LYS
1	D	321	PHE
1	D	324	PHE
1	D	340	GLN
1	D	348	VAL
1	D	354	VAL
1	D	364	LEU
1	B	23	ASP
1	B	37	LEU
1	B	59	ASP
1	B	101	THR
1	B	108	LEU
1	B	112	LEU
1	B	134	LEU
1	B	138	GLU
1	B	156	LEU
1	B	221	ILE
1	B	225	LEU
1	B	231	LEU
1	B	272	THR
1	B	276	PHE
1	B	300	ARG
1	B	321	PHE
1	B	331	GLN
1	B	348	VAL
1	B	354	VAL
1	B	364	LEU
1	B	382	LEU
1	B	387	GLU
1	C	16	VAL
1	C	17	SER
1	C	25	SER
1	C	37	LEU
1	C	66	MET
1	C	98	ILE
1	C	101	THR
1	C	108	LEU
1	C	112	LEU
1	C	144	THR
1	C	152	THR

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Mol	Chain	Res	Type
1	C	156	LEU
1	C	161	LEU
1	C	163	GLU
1	C	216	GLU
1	C	231	LEU
1	C	246	LEU
1	C	267	VAL
1	C	272	THR
1	C	300	ARG
1	C	305	GLU
1	C	321	PHE
1	C	348	VAL
1	C	354	VAL
1	C	361	GLU
1	C	364	LEU
1	C	374	THR
1	C	382	LEU
1	C	388	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	390/393 (99%)	0.14	6 (1%) 76 75	8, 20, 40, 58	0
1	B	382/393 (97%)	0.39	20 (5%) 31 30	11, 24, 51, 70	0
1	C	388/393 (98%)	0.25	8 (2%) 67 65	12, 25, 43, 72	0
1	D	377/393 (95%)	0.70	43 (11%) 7 6	15, 33, 64, 73	0
All	All	1537/1572 (97%)	0.37	77 (5%) 32 32	8, 25, 55, 73	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	TYR	6.2
1	D	330	ALA	6.0
1	D	375	ILE	5.8
1	D	315	ILE	5.5
1	B	331	GLN	5.5
1	D	16	VAL	5.5
1	B	332	GLY	5.1
1	D	313	LYS	4.8
1	A	62	HIS	4.5
1	D	382	LEU	4.4
1	D	304	ILE	4.3
1	D	314	ILE	4.3
1	D	378	ALA	4.3
1	B	389	TYR	4.1
1	D	386	MET	4.1
1	B	329	VAL	4.0
1	D	332	GLY	3.9
1	C	62	HIS	3.7
1	D	379	MET	3.6
1	D	341	ASP	3.6
1	B	330	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	311	LYS	3.4
1	D	19	ILE	3.2
1	D	68	GLY	3.2
1	B	19	ILE	3.1
1	D	331	GLN	3.0
1	D	312	PHE	3.0
1	D	336	PHE	3.0
1	D	15	GLU	2.9
1	A	63	TYR	2.9
1	D	309	ALA	2.8
1	D	18	MET	2.8
1	C	61	SER	2.8
1	C	327	ILE	2.7
1	A	389	TYR	2.7
1	D	349	ALA	2.7
1	D	385	PHE	2.7
1	B	328	PRO	2.7
1	B	338	PHE	2.7
1	D	265	TYR	2.6
1	B	320	ALA	2.6
1	D	303	ILE	2.6
1	D	335	SER	2.6
1	D	328	PRO	2.6
1	D	320	ALA	2.6
1	C	309	ALA	2.5
1	C	314	ILE	2.5
1	D	307	MET	2.5
1	D	338	PHE	2.4
1	B	294	GLU	2.4
1	B	313	LYS	2.4
1	B	386	MET	2.4
1	D	354	VAL	2.3
1	D	292	MET	2.3
1	D	33	LEU	2.3
1	D	161	LEU	2.3
1	B	25	SER	2.3
1	B	28	ASP	2.3
1	B	22	PHE	2.2
1	B	387	GLU	2.2
1	D	339	LEU	2.2
1	A	337	LYS	2.2
1	B	27	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	390	ALA	2.1
1	B	18	MET	2.1
1	D	302	TYR	2.1
1	B	67	ALA	2.1
1	A	61	SER	2.1
1	D	344	LYS	2.1
1	B	364	LEU	2.1
1	D	369	ALA	2.1
1	D	371	SER	2.1
1	D	296	TYR	2.1
1	D	376	LYS	2.0
1	C	328	PRO	2.0
1	D	32	VAL	2.0
1	C	16	VAL	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.