Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:12 PM GMT

PDB ID	:	4R8F
Title	:	Crystal structure of yeast aminopeptidase 1 (Ape1)
Authors	:	Su, M.-Y.; Chang, C.-I.
Deposited on	:	2014-09-02
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

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 2.50 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.
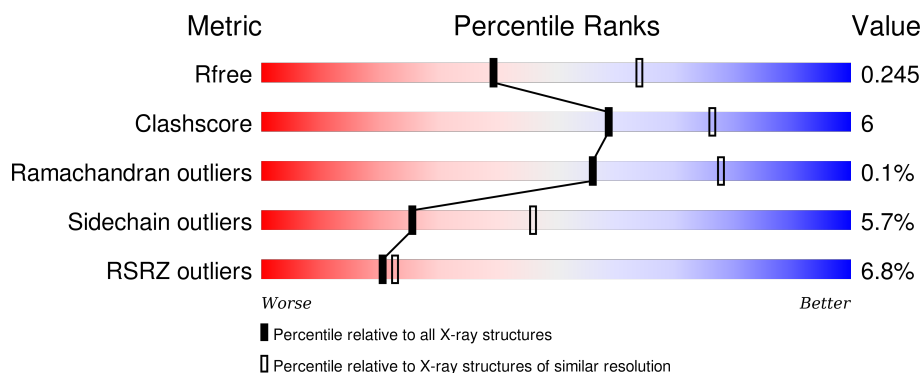
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	470	
1	B	470	
1	C	470	
1	D	470	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13635 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 Vacuolar aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total 3418	C 2188	N 577	O 645	S 8	0	0	0
1	B	428	Total 3340	C 2142	N 564	O 626	S 8	0	0	0
1	C	437	Total 3414	C 2189	N 576	O 641	S 8	0	0	0
1	D	432	Total 3372	C 2162	N 567	O 635	S 8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P14904
B	1	MET	-	EXPRESSION TAG	UNP P14904
C	1	MET	-	EXPRESSION TAG	UNP P14904
D	1	MET	-	EXPRESSION TAG	UNP P14904

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total 25	O 25	0	0
2	B	20	Total 20	O 20	0	0
2	C	27	Total 27	O 27	0	0
2	D	19	Total 19	O 19	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: Vacuolar aminopeptidase 1

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Q303 G304 A305 K324 P325 N334 D341 V342 L345 F350 P351 E352 V353 Y354 L355 K356 N357 H358 L368 S369 L370 V380 E387 R392 Q401 I402 LYS ASN ASN SER ARG SER GLY G410 T411 L427 Q431 L432 S433 M434 H435 V446 R461 E466

L470

• Molecule 1: Vacuolar aminopeptidase 1

7%

Chain D:

75%   15%   •   8%

MET GLU HIS N4 F15 I16 S27 L33 L41 S42 E43 K44 S45 Q48 K57 R62 N63 N66 N75 W76 R77 V89 T93 V94 K97 P98 V99 D103 T104 A105 E106 G107 Y108 G109 R110 V113 G118 T119 L120 N143 C158 R159

L163 ALA P165 H166 F167 GLY LYS PRO ALA GLU GLY PRO F175 D176 K177 E178 ASP Q180 T181 I182 P183 V184 ILE GLY PHE PRO THR PRO ASP GLU GLY ASN E196 P197 D200 D201 S205 H214 S228 Q232 D239 T244 R257 L258 D259 D260 R261 M268 I272

A275 M279 E282 F286 I297 Q303 E315 K323 K324 P325 L328 V342 N343 H344 L345 Y346 N347 P348 N349 F350 PRO GLU VAL TYR LEU LYS ASN HIS F359 P360 T367 L370 D371 P372 N373 V380 E387 Q401 I402 LYS ASN ASN SER ARG SER

GLY G410 T411 L427 M434 H435 L470

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	140.17Å 140.17Å 348.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	116.23 – 2.50 19.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (116.23-2.50) 95.9 (19.92-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.215 , 0.246 0.217 , 0.245	Depositor DCC
R_{free} test set	4219 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 46.5	EDS
Estimated twinning fraction	0.011 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.015 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.009 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.015 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.011 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.014 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.038 for -h-k,k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 84889 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13635	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.31	0/3493	0.59	0/4729
1	B	0.30	0/3413	0.55	0/4619
1	C	0.30	0/3489	0.55	0/4723
1	D	0.30	0/3444	0.56	0/4656
All	All	0.30	0/13839	0.56	0/18727

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	352	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3418	0	3387	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3340	0	3318	40	0
1	C	3414	0	3384	51	0
1	D	3372	0	3337	49	0
2	A	25	0	0	1	0
2	B	20	0	0	3	0
2	C	27	0	0	0	0
2	D	19	0	0	0	0
All	All	13635	0	13426	157	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 6.

All (157) 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:380:VAL:CG2	1:C:234:ASP:HB2	2.05	0.86
1:B:380:VAL:CG1	1:C:232:GLN:HB3	2.12	0.79
1:B:232:GLN:HB3	1:D:380:VAL:CG2	2.15	0.77
1:A:7:ASP:HA	1:A:9:ALA:H	1.49	0.77
1:D:315:GLU:HG3	1:D:328:LEU:HD21	1.68	0.75
1:C:392:ARG:NH2	1:C:466:GLU:OE2	2.21	0.74
1:A:6:GLU:C	1:A:8:ILE:HG22	2.08	0.73
1:B:158:CYS:HB2	1:B:182:ILE:HG22	1.70	0.72
1:D:158:CYS:SG	1:D:182:ILE:HG21	2.29	0.72
1:D:158:CYS:HB2	1:D:182:ILE:HG22	1.71	0.72
1:A:7:ASP:OD1	1:A:7:ASP:N	2.28	0.67
1:C:158:CYS:HB2	1:C:182:ILE:HG22	1.78	0.66
1:B:425:ILE:HG22	2:B:516:HOH:O	1.95	0.65
1:D:89:VAL:O	1:D:261:ARG:NH1	2.31	0.64
1:B:355:LEU:O	1:B:359:PHE:CD2	2.51	0.63
1:A:239:ASP:O	1:A:257:ARG:NH2	2.32	0.63
1:C:345:LEU:HB3	1:C:432:LEU:HD12	1.81	0.61
1:D:158:CYS:HB2	1:D:182:ILE:CG2	2.31	0.61
1:B:113:VAL:HG21	1:B:182:ILE:HD11	1.82	0.60
1:C:113:VAL:HG22	1:C:182:ILE:HD11	1.83	0.59
1:A:77:ARG:HH11	1:A:77:ARG:HG2	1.67	0.59
1:A:158:CYS:SG	1:A:182:ILE:HG21	2.41	0.59
1:C:342:VAL:HG11	1:C:431:GLN:NE2	2.18	0.59
1:B:380:VAL:HG22	1:C:234:ASP:HB2	1.85	0.58
1:B:297:ILE:HG21	1:D:373:ASN:HA	1.84	0.58
1:C:158:CYS:SG	1:C:182:ILE:HG21	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:VAL:CG2	1:D:232:GLN:HB3	2.33	0.58
1:D:347:ASN:OD1	1:D:348:PRO:HD2	2.02	0.58
1:D:239:ASP:O	1:D:257:ARG:NH2	2.37	0.56
1:B:158:CYS:HB2	1:B:182:ILE:CG2	2.35	0.56
1:C:113:VAL:CG2	1:C:182:ILE:HD11	2.35	0.56
1:C:380:VAL:HG22	1:D:232:GLN:HB3	1.86	0.56
1:C:334:ASN:O	1:C:461:ARG:NH2	2.39	0.56
1:B:355:LEU:O	1:B:359:PHE:HD2	1.88	0.55
1:D:158:CYS:SG	1:D:182:ILE:CG2	2.94	0.55
1:D:43:GLU:OE1	1:D:62:ARG:HG3	2.07	0.55
1:D:119:THR:CG2	1:D:120:LEU:N	2.70	0.55
1:D:166:HIS:O	1:D:167:PHE:CD2	2.59	0.55
1:A:7:ASP:HA	1:A:9:ALA:N	2.17	0.55
1:A:54:ASP:O	1:A:280:THR:HG23	2.06	0.55
1:B:196:GLU:HB3	1:B:197:PRO:HD3	1.88	0.54
1:D:57:LYS:NZ	1:D:275:ALA:O	2.41	0.54
1:D:342:VAL:HG23	1:D:434:MET:SD	2.48	0.54
1:D:165:PRO:HA	1:D:166:HIS:C	2.27	0.53
1:C:62:ARG:HB3	1:C:66:ASN:HB3	1.91	0.53
1:D:165:PRO:HA	1:D:166:HIS:O	2.09	0.53
1:C:182:ILE:N	1:C:182:ILE:HD12	2.24	0.53
1:A:181:THR:HA	1:A:182:ILE:HD12	1.91	0.53
1:A:181:THR:HG22	1:A:182:ILE:H	1.74	0.52
1:C:461:ARG:HD3	1:C:461:ARG:O	2.10	0.52
1:A:6:GLU:C	1:A:7:ASP:OD1	2.49	0.51
1:B:370:LEU:HB2	1:B:401:GLN:HG2	1.93	0.51
1:C:358:HIS:CE1	1:D:99:VAL:HB	2.45	0.51
1:D:258:LEU:O	1:D:260:ASP:HA	2.11	0.51
1:D:75:ASN:O	1:D:77:ARG:NH1	2.44	0.51
1:D:48:GLN:HE22	1:D:323:LYS:CE	2.23	0.51
1:D:180:GLN:O	1:D:181:THR:HG22	2.11	0.51
1:A:158:CYS:HB2	1:A:182:ILE:CG2	2.41	0.50
1:A:113:VAL:HG21	1:A:182:ILE:HD11	1.93	0.50
1:A:161:PRO:HD3	1:A:183:PRO:HD2	1.92	0.50
1:B:210:LYS:HB2	1:B:211:HIS:CD2	2.47	0.50
1:B:380:VAL:HG11	1:C:232:GLN:HB3	1.92	0.50
1:B:380:VAL:HG21	1:C:234:ASP:HB2	1.90	0.50
1:D:48:GLN:HE22	1:D:323:LYS:HE3	1.77	0.49
1:B:357:ASN:HB3	1:C:99:VAL:HG11	1.93	0.49
1:A:358:HIS:HB3	1:A:401:GLN:H	1.77	0.49
1:C:219:VAL:HG21	1:C:233:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:HIS:HB3	1:B:412:ILE:HD11	1.95	0.49
1:C:292:TYR:CE1	1:C:305:ALA:HA	2.48	0.48
1:C:211:HIS:HB2	1:C:216:LEU:HD21	1.94	0.48
1:D:360:PRO:HG3	1:D:367:THR:HG21	1.94	0.48
1:A:196:GLU:HB3	1:A:197:PRO:HD3	1.96	0.48
1:C:97:LYS:HD2	1:C:112:ALA:HB1	1.96	0.48
1:B:135:LEU:HD12	1:B:223:ALA:HB2	1.95	0.48
1:D:62:ARG:HB3	1:D:66:ASN:HB3	1.96	0.48
1:C:260:ASP:OD2	1:C:341:ASP:HA	2.14	0.48
1:A:395:ASP:OD1	1:A:451:LYS:HE3	2.14	0.48
1:B:118:GLY:HA3	1:B:120:LEU:HD13	1.96	0.48
1:C:109:GLY:HA3	1:C:185:ILE:CG1	2.43	0.48
1:D:113:VAL:CG2	1:D:182:ILE:HD11	2.45	0.47
1:B:355:LEU:O	1:B:359:PHE:CE2	2.67	0.47
1:B:63:ASN:HB3	1:B:303:GLN:HG2	1.96	0.47
1:C:181:THR:HG22	1:C:182:ILE:H	1.80	0.47
1:B:158:CYS:SG	1:B:182:ILE:HG21	2.55	0.47
1:B:380:VAL:HG12	1:C:232:GLN:HB3	1.96	0.47
1:D:119:THR:HG23	1:D:120:LEU:N	2.30	0.47
1:A:358:HIS:ND1	1:A:401:GLN:HB2	2.30	0.47
1:B:232:GLN:HB3	1:D:380:VAL:HG21	1.93	0.46
1:B:370:LEU:HD13	1:C:98:PRO:HG2	1.97	0.46
1:D:370:LEU:O	1:D:401:GLN:HA	2.15	0.46
1:A:7:ASP:CA	1:A:9:ALA:H	2.24	0.46
1:B:427:LEU:HD23	2:B:516:HOH:O	2.14	0.46
1:C:260:ASP:CG	1:C:342:VAL:HG13	2.35	0.46
1:D:16:ILE:HD11	1:D:261:ARG:HB2	1.97	0.46
1:B:119:THR:H	1:B:120:LEU:HA	1.81	0.46
1:C:370:LEU:HB2	1:C:401:GLN:HG2	1.99	0.45
1:B:370:LEU:HD13	1:C:98:PRO:CG	2.47	0.45
1:D:344:HIS:O	1:D:360:PRO:HD2	2.16	0.45
1:D:113:VAL:HG21	1:D:182:ILE:HD11	1.98	0.45
1:A:355:LEU:CD2	1:A:358:HIS:CD2	3.00	0.45
1:D:94:VAL:HG22	1:D:120:LEU:HD13	1.99	0.44
1:C:239:ASP:O	1:C:257:ARG:NH2	2.51	0.44
1:A:434:MET:HE2	2:A:509:HOH:O	2.16	0.44
1:C:259:ASP:HA	1:C:260:ASP:HA	1.71	0.44
1:A:259:ASP:HA	1:A:260:ASP:HA	1.72	0.44
1:B:260:ASP:OD1	1:B:342:VAL:HG23	2.17	0.44
1:B:109:GLY:C	1:B:184:VAL:HG22	2.38	0.44
1:A:158:CYS:HB2	1:A:182:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:CG2	1:A:182:ILE:HD11	2.48	0.44
1:B:391:ARG:NH2	1:C:206:PRO:HB3	2.33	0.43
1:D:324:LYS:HE3	1:D:325:PRO:O	2.17	0.43
1:D:33:LEU:HD21	1:D:268:MET:HE3	1.99	0.43
1:D:165:PRO:HA	1:D:166:HIS:CB	2.47	0.43
1:A:7:ASP:N	1:A:8:ILE:HG22	2.34	0.43
1:D:119:THR:HG23	1:D:120:LEU:H	1.83	0.43
1:A:370:LEU:O	1:A:401:GLN:HA	2.18	0.43
1:C:355:LEU:HD11	1:D:97:LYS:HZ1	1.82	0.43
1:A:162:SER:O	1:C:433:SER:HB3	2.18	0.43
1:D:163:LEU:HD23	1:D:167:PHE:CE2	2.53	0.43
1:D:359:PHE:HA	1:D:360:PRO:HD3	1.92	0.43
1:B:119:THR:N	1:B:120:LEU:HA	2.34	0.42
1:B:370:LEU:O	1:B:401:GLN:HG2	2.20	0.42
1:C:138:LYS:HD3	1:C:143:ASN:HA	2.01	0.42
1:A:438:ARG:O	1:C:159:ARG:NH2	2.52	0.42
1:B:425:ILE:CG2	2:B:516:HOH:O	2.61	0.42
1:A:371:ASP:OD1	1:A:372:PRO:HD2	2.20	0.42
1:C:461:ARG:C	1:C:461:ARG:HD3	2.39	0.42
1:D:158:CYS:CB	1:D:182:ILE:CG2	2.98	0.42
1:D:360:PRO:HG3	1:D:367:THR:CG2	2.49	0.42
1:A:371:ASP:CG	1:A:373:ASN:O	2.58	0.42
1:C:350:PHE:N	1:C:351:PRO:CD	2.82	0.42
1:B:387:GLU:OE2	1:C:232:GLN:NE2	2.47	0.42
1:D:372:PRO:O	1:D:373:ASN:HB2	2.20	0.42
1:C:76:TRP:CD1	1:C:286:PHE:HB2	2.55	0.41
1:C:262:LEU:CD1	1:C:446:VAL:HG22	2.49	0.41
1:A:150:VAL:HG22	1:A:222:LEU:HB2	2.03	0.41
1:A:128:ASP:HB3	1:A:156:PRO:HB3	2.02	0.41
1:C:219:VAL:HG21	1:C:233:MET:HE2	2.01	0.41
1:C:260:ASP:OD1	1:C:342:VAL:HG13	2.21	0.41
1:B:259:ASP:HA	1:B:260:ASP:HA	1.75	0.41
1:D:63:ASN:CB	1:D:303:GLN:HG2	2.51	0.41
1:A:163:LEU:HD21	1:C:353:VAL:HG21	2.03	0.41
1:B:199:THR:HG22	1:B:200:ASP:N	2.36	0.41
1:C:181:THR:HA	1:C:182:ILE:HD12	2.02	0.41
1:C:63:ASN:HB3	1:C:303:GLN:HG2	2.02	0.41
1:B:262:LEU:CD1	1:B:446:VAL:HG22	2.50	0.41
1:D:205:SER:HB2	1:D:228:SER:HA	2.02	0.41
1:D:349:ASN:N	1:D:349:ASN:OD1	2.54	0.41
1:A:182:ILE:N	1:A:182:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:TYR:CE1	1:A:305:ALA:HA	2.56	0.41
1:A:88:HIS:NE2	1:A:260:ASP:HB2	2.35	0.40
1:A:205:SER:HB2	1:A:228:SER:HA	2.04	0.40
1:D:402:ILE:HG22	1:D:402:ILE:O	2.22	0.40
1:C:368:LEU:HD12	1:C:427:LEU:HD23	2.02	0.40
1:A:248:ILE:HG22	1:C:185:ILE:CG2	2.52	0.40
1:B:124:TRP:CE3	1:B:437:ILE:HD12	2.57	0.40
1:A:402:ILE:HD12	1:A:402:ILE:N	2.37	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	430/470 (92%)	425 (99%)	4 (1%)	1 (0%)	52	75
1	B	418/470 (89%)	413 (99%)	5 (1%)	0	100	100
1	C	427/470 (91%)	420 (98%)	7 (2%)	0	100	100
1	D	418/470 (89%)	410 (98%)	8 (2%)	0	100	100
All	All	1693/1880 (90%)	1668 (98%)	24 (1%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	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	370/396 (93%)	348 (94%)	22 (6%)	24	44
1	B	362/396 (91%)	347 (96%)	15 (4%)	37	63
1	C	370/396 (93%)	353 (95%)	17 (5%)	33	57
1	D	365/396 (92%)	335 (92%)	30 (8%)	14	27
All	All	1467/1584 (93%)	1383 (94%)	84 (6%)	25	46

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	7	ASP
1	A	43	GLU
1	A	77	ARG
1	A	104	THR
1	A	120	LEU
1	A	123	LEU
1	A	134	ARG
1	A	159	ARG
1	A	177	LYS
1	A	178	GLU
1	A	212	CYS
1	A	221	LYS
1	A	280	THR
1	A	286	PHE
1	A	323	LYS
1	A	326	VAL
1	A	385	LEU
1	A	387	GLU
1	A	401	GLN
1	A	431	GLN
1	A	470	LEU
1	B	74	LYS
1	B	77	ARG
1	B	93	THR
1	B	122	GLU
1	B	142	THR
1	B	180	GLN
1	B	181	THR
1	B	281	GLU

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Mol	Chain	Res	Type
1	B	286	PHE
1	B	343	ASN
1	B	352	GLU
1	B	355	LEU
1	B	385	LEU
1	B	414	PRO
1	B	470	LEU
1	C	14	ASP
1	C	21	THR
1	C	93	THR
1	C	103	ASP
1	C	104	THR
1	C	159	ARG
1	C	163	LEU
1	C	212	CYS
1	C	221	LYS
1	C	244	THR
1	C	248	ILE
1	C	286	PHE
1	C	303	GLN
1	C	387	GLU
1	C	411	THR
1	C	433	SER
1	C	461	ARG
1	D	4	ASN
1	D	15	PHE
1	D	27	SER
1	D	41	LEU
1	D	45	SER
1	D	93	THR
1	D	104	THR
1	D	110	ARG
1	D	119	THR
1	D	143	ASN
1	D	159	ARG
1	D	167	PHE
1	D	178	GLU
1	D	180	GLN
1	D	181	THR
1	D	184	VAL
1	D	244	THR
1	D	272	ILE

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Mol	Chain	Res	Type
1	D	279	ASN
1	D	286	PHE
1	D	297	ILE
1	D	303	GLN
1	D	324	LYS
1	D	328	LEU
1	D	343	ASN
1	D	345	LEU
1	D	360	PRO
1	D	387	GLU
1	D	411	THR
1	D	427	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	ASN
1	B	66	ASN
1	C	343	ASN
1	C	431	GLN
1	D	48	GLN
1	D	143	ASN
1	D	303	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	438/470 (93%)	0.07	27 (6%)	24	27	20, 34, 73, 103	0
1	B	428/470 (91%)	0.06	26 (6%)	25	27	23, 38, 75, 93	0
1	C	437/470 (92%)	0.08	30 (6%)	20	22	24, 36, 73, 102	0
1	D	432/470 (91%)	0.16	35 (8%)	15	16	24, 41, 75, 109	0
All	All	1735/1880 (92%)	0.09	118 (6%)	20	23	20, 37, 75, 109	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	HIS	6.9
1	A	5	TYR	6.5
1	D	410	GLY	5.5
1	B	410	GLY	5.5
1	A	410	GLY	5.0
1	A	3	HIS	4.8
1	C	353	VAL	4.6
1	D	167	PHE	4.5
1	B	101	PHE	4.5
1	A	197	PRO	4.4
1	D	175	PHE	4.4
1	B	119	THR	4.2
1	C	107	GLY	4.1
1	A	325	PRO	4.1
1	C	104	THR	4.1
1	D	349	ASN	4.1
1	D	106	GLU	4.0
1	A	119	THR	3.9
1	B	355	LEU	3.9
1	B	200	ASP	3.9
1	A	4	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	107	GLY	3.8
1	A	179	ASP	3.8
1	D	348	PRO	3.8
1	D	118	GLY	3.7
1	A	105	ALA	3.7
1	D	325	PRO	3.7
1	D	359	PHE	3.6
1	C	106	GLU	3.6
1	C	195	ASN	3.6
1	C	167	PHE	3.6
1	C	119	THR	3.6
1	C	355	LEU	3.6
1	B	110	ARG	3.5
1	B	203	LYS	3.5
1	B	120	LEU	3.5
1	D	371	ASP	3.4
1	D	119	THR	3.4
1	C	163	LEU	3.3
1	C	103	ASP	3.3
1	C	352	GLU	3.3
1	C	105	ALA	3.3
1	B	356	LYS	3.3
1	C	180	GLN	3.3
1	A	200	ASP	3.2
1	D	104	THR	3.2
1	A	350	PHE	3.2
1	D	196	GLU	3.2
1	A	106	GLU	3.2
1	A	104	THR	3.2
1	C	356	LYS	3.1
1	B	141	GLY	3.1
1	B	102	LYS	3.1
1	B	281	GLU	3.0
1	D	120	LEU	3.0
1	A	178	GLU	3.0
1	D	176	ASP	3.0
1	C	325	PRO	3.0
1	D	197	PRO	3.0
1	B	109	GLY	2.9
1	D	163	LEU	2.9
1	D	435	HIS	2.8
1	A	164	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	103	ASP	2.8
1	C	214	HIS	2.7
1	B	107	GLY	2.7
1	B	209	GLY	2.7
1	C	281	GLU	2.7
1	B	118	GLY	2.7
1	B	351	PRO	2.7
1	A	141	GLY	2.7
1	D	350	PHE	2.7
1	A	103	ASP	2.6
1	A	107	GLY	2.6
1	A	352	GLU	2.6
1	B	4	ASN	2.6
1	D	105	ALA	2.5
1	B	184	VAL	2.5
1	D	279	ASN	2.5
1	B	180	GLN	2.5
1	B	435	HIS	2.5
1	D	346	TYR	2.5
1	C	435	HIS	2.5
1	D	166	HIS	2.5
1	D	165	PRO	2.5
1	D	282	GLU	2.5
1	B	143	ASN	2.4
1	C	279	ASN	2.4
1	A	196	GLU	2.4
1	C	357	ASN	2.4
1	D	177	LYS	2.4
1	B	140	LYS	2.3
1	C	324	LYS	2.3
1	B	352	GLU	2.3
1	D	343	ASN	2.3
1	C	199	THR	2.3
1	C	200	ASP	2.3
1	D	214	HIS	2.3
1	C	108	TYR	2.3
1	B	374	GLY	2.3
1	A	180	GLN	2.3
1	A	353	VAL	2.2
1	D	178	GLU	2.2
1	C	143	ASN	2.2
1	A	277	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	354	TYR	2.2
1	D	181	THR	2.2
1	B	201	ASP	2.2
1	C	209	GLY	2.1
1	A	208	PHE	2.1
1	C	141	GLY	2.1
1	D	108	TYR	2.1
1	A	279	ASN	2.1
1	C	4	ASN	2.1
1	D	200	ASP	2.0
1	C	354	TYR	2.0
1	D	201	ASP	2.0
1	A	108	TYR	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.