Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:10 PM GMT

PDB ID	:	1J3U
Title	:	Crystal structure of aspartase from Bacillus sp. YM55-1
Authors	:	Fujii, T.; Sakai, H.; Kawata, Y.; Hata, Y.
Deposited on	:	2003-02-16
Resolution	:	2.50 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 ⓘ) were used in the production of this report:

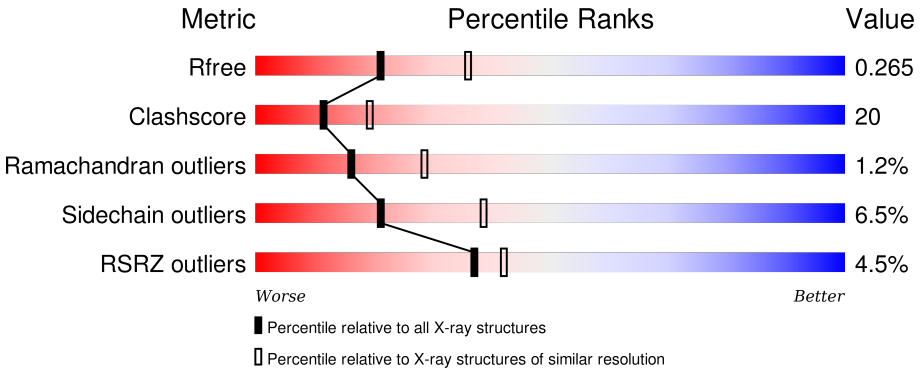
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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	468	5% 62% 34%
1	B	468	4% 60% 36%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7245 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 aspartase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3513	2211	596	684	22			
1	B	462	Total	C	N	O	S	0	0	0
			3519	2217	596	684	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ILE	THR	CONFLICT	UNP Q9LCC6
B	460	ILE	THR	CONFLICT	UNP Q9LCC6

- Molecule 2 is water.

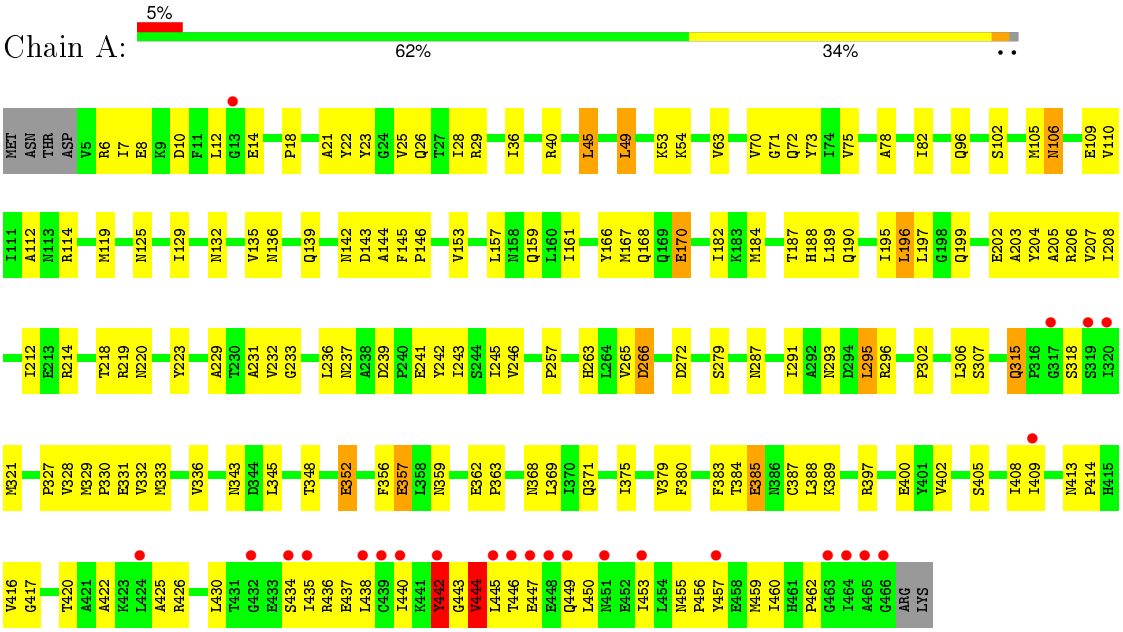
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		
2	B	89	Total	O	0	0
			89	89		

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.

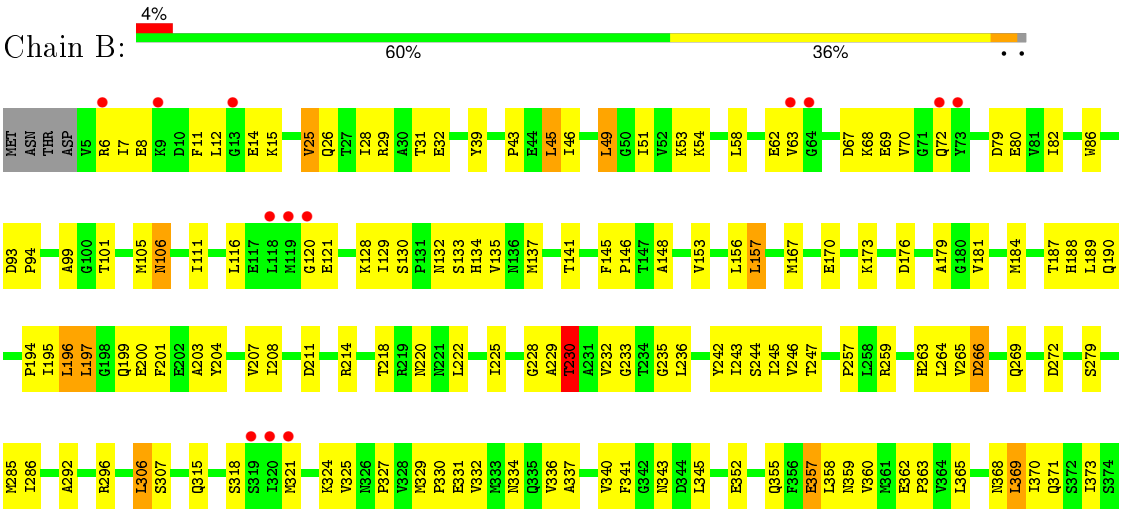
- Molecule 1: aspartase

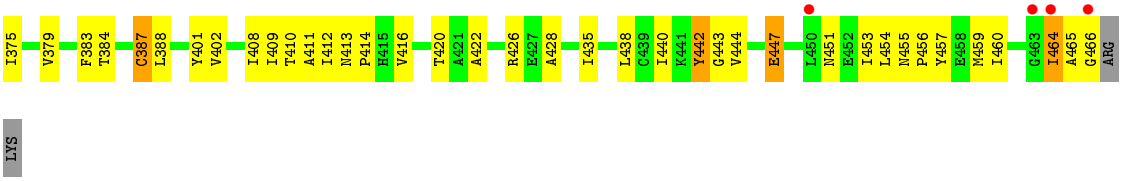
Chain A:



- Molecule 1: aspartase

Chain B:




I375
V379
F383
T384
C387
L388
Y401
V402
I408
I409
T410
A411
I412
N413
P414
K415
V416
T420
A421
A422
R426
E427
A428
I435
L438
C439
I440
K441
Y442
G443
V444
E447
L450
N451
E452
I453
L454
N455
P456
Y457
E458
N459
I460
G463
I464
A465
G466
ARG
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.90Å 139.40Å 100.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.11 – 2.50 59.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.0 (55.11-2.50) 90.1 (59.99-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.266 0.221 , 0.265	Depositor DCC
R_{free} test set	1653 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.832	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 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	1 of 33759 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7245	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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	0.37	0/3571	0.57	0/4844
1	B	0.34	0/3577	0.55	0/4852
All	All	0.35	0/7148	0.56	0/9696

There are no bond length outliers.

There are no bond angle outliers.

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	3513	0	3457	147	0
1	B	3519	0	3475	152	0
2	A	124	0	0	6	1
2	B	89	0	0	4	2
All	All	7245	0	6932	285	2

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 20.

All (285) 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:229:ALA:HB1	1:B:233:GLY:HA2	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HD11	1:A:14:GLU:HB3	1.47	0.93
1:A:336:VAL:HG21	1:A:379:VAL:HG11	1.51	0.91
1:B:6:ARG:HG2	1:B:7:ILE:H	1.40	0.87
1:B:184:MET:HE1	1:B:194:PRO:HG3	1.54	0.86
1:A:408:ILE:HG21	1:A:435:ILE:HG21	1.58	0.85
1:B:336:VAL:HG21	1:B:379:VAL:HG11	1.56	0.85
1:A:343:ASN:HD21	1:A:371:GLN:HE21	1.27	0.83
1:A:170:GLU:HG3	2:A:563:HOH:O	1.80	0.82
1:B:196:LEU:HD23	1:B:460:ILE:HG21	1.60	0.81
1:A:408:ILE:CG2	1:A:435:ILE:HG21	2.13	0.79
1:B:26:GLN:NE2	1:B:105:MET:HG3	1.99	0.78
1:B:43:PRO:HA	1:B:46:ILE:HD12	1.66	0.77
1:A:184:MET:HE3	1:A:402:VAL:HA	1.66	0.76
1:A:184:MET:CE	1:A:402:VAL:HA	2.15	0.76
1:A:291:ILE:O	1:A:295:LEU:HD22	1.86	0.75
1:A:196:LEU:HB2	1:A:460:ILE:HD13	1.66	0.75
1:A:96:GLN:NE2	1:A:102:SER:HB2	2.01	0.75
1:B:416:VAL:HG12	1:B:420:THR:HB	1.68	0.75
1:B:51:ILE:HA	1:B:82:ILE:HD11	1.69	0.74
1:B:8:GLU:HB2	1:B:25:VAL:HG13	1.69	0.74
1:A:413:ASN:HB3	1:A:414:PRO:HD3	1.68	0.73
1:A:438:LEU:O	1:A:442:TYR:HB2	1.88	0.73
1:B:464:ILE:HG12	1:B:465:ALA:H	1.53	0.72
1:B:70:VAL:HG13	1:B:129:ILE:HG12	1.71	0.72
1:A:229:ALA:HB1	1:A:233:GLY:HA2	1.72	0.71
1:B:99:ALA:HB2	1:B:360:VAL:HA	1.73	0.70
1:A:443:GLY:O	1:A:444:VAL:HG13	1.91	0.70
1:B:187:THR:O	1:B:188:HIS:HB2	1.91	0.70
1:A:436:ARG:HG3	1:A:450:LEU:HD23	1.74	0.69
1:A:7:ILE:CD1	1:A:14:GLU:HB3	2.22	0.69
1:B:7:ILE:HD11	1:B:14:GLU:OE2	1.94	0.68
1:A:96:GLN:HE22	1:A:102:SER:HB2	1.58	0.68
1:A:359:ASN:O	1:A:362:GLU:HG3	1.94	0.67
1:B:327:PRO:O	1:B:330:PRO:HD2	1.95	0.67
1:B:438:LEU:O	1:B:442:TYR:HB2	1.95	0.67
1:B:336:VAL:HG21	1:B:379:VAL:CG1	2.24	0.66
1:A:455:ASN:ND2	1:A:456:PRO:HD2	2.10	0.66
1:B:101:THR:HA	1:B:141:THR:HG21	1.77	0.66
1:A:449:GLN:HB2	2:A:650:HOH:O	1.94	0.66
1:B:121:GLU:OE1	1:B:128:LYS:HE2	1.95	0.66
1:B:184:MET:HE1	1:B:194:PRO:CG	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE2	1:A:402:VAL:HG22	1.77	0.65
1:B:359:ASN:O	1:B:362:GLU:HG3	1.97	0.65
1:A:343:ASN:HD21	1:A:371:GLN:NE2	1.95	0.65
1:B:68:LYS:O	1:B:72:GLN:HB2	1.97	0.64
1:A:327:PRO:O	1:A:331:GLU:HG3	1.97	0.64
1:B:447:GLU:O	1:B:451:ASN:ND2	2.31	0.64
1:B:196:LEU:CG	1:B:460:ILE:HD13	2.27	0.64
1:A:22:TYR:O	1:A:110:VAL:HA	1.98	0.64
1:B:196:LEU:HG	1:B:460:ILE:HD13	1.78	0.64
1:B:188:HIS:O	1:B:189:LEU:HB2	1.98	0.64
1:A:214:ARG:O	1:A:218:THR:HG23	1.98	0.64
1:A:63:VAL:HG12	1:A:63:VAL:O	1.98	0.63
1:B:230:THR:HG21	1:B:236:LEU:O	1.97	0.63
1:B:184:MET:HE3	1:B:402:VAL:HG13	1.81	0.62
1:A:384:THR:HA	1:A:388:LEU:HB3	1.82	0.62
1:A:459:MET:O	1:B:236:LEU:HD13	2.00	0.61
1:A:7:ILE:HD11	1:A:14:GLU:CB	2.27	0.61
1:B:196:LEU:HD23	1:B:460:ILE:HD13	1.81	0.61
1:B:70:VAL:CG1	1:B:129:ILE:HG12	2.30	0.61
1:B:440:ILE:HD11	1:B:447:GLU:HG2	1.83	0.60
1:B:220:ASN:HB2	2:B:545:HOH:O	2.00	0.60
1:B:196:LEU:CD2	1:B:460:ILE:HD13	2.31	0.60
1:A:187:THR:O	1:A:188:HIS:HB2	2.01	0.60
1:A:362:GLU:N	1:A:363:PRO:HD2	2.17	0.60
1:A:70:VAL:HG22	1:A:119:MET:HE3	1.83	0.60
1:A:263:HIS:CE1	1:A:265:VAL:HB	2.37	0.60
1:B:456:PRO:O	1:B:460:ILE:HG12	2.03	0.59
1:A:456:PRO:O	1:A:460:ILE:HG12	2.02	0.59
1:B:106:ASN:HD22	1:B:106:ASN:C	2.06	0.59
1:A:436:ARG:HG3	1:A:450:LEU:CD2	2.32	0.59
1:B:343:ASN:HD21	1:B:371:GLN:HE21	1.50	0.59
1:A:336:VAL:HG21	1:A:379:VAL:CG1	2.31	0.58
1:B:329:MET:HB2	1:B:330:PRO:HD3	1.83	0.58
1:A:380:PHE:O	1:A:384:THR:HG23	2.03	0.58
1:B:428:ALA:HB2	1:B:438:LEU:HD22	1.85	0.58
1:A:455:ASN:HD22	1:A:456:PRO:HD2	1.68	0.58
1:B:375:ILE:O	1:B:379:VAL:HG22	2.03	0.58
1:B:6:ARG:HG2	1:B:7:ILE:N	2.16	0.58
1:A:279:SER:HB3	1:B:279:SER:HB3	1.85	0.58
1:A:167:MET:CE	1:A:380:PHE:HA	2.35	0.57
1:B:49:LEU:HD13	1:B:148:ALA:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:MET:HB2	1:B:384:THR:HG21	1.87	0.57
1:B:157:LEU:HD13	1:B:373:ILE:HD13	1.87	0.57
1:A:293:ASN:HA	1:A:296:ARG:NH1	2.20	0.56
1:B:343:ASN:HA	1:B:368:ASN:HD22	1.70	0.56
1:A:232:VAL:CG1	1:B:195:ILE:HD12	2.34	0.56
1:A:409:ILE:HG12	1:A:425:ALA:HB2	1.86	0.56
1:B:329:MET:O	1:B:332:VAL:HG12	2.05	0.56
1:A:318:SER:CB	1:A:321:MET:HB3	2.36	0.56
1:A:236:LEU:HD13	1:B:459:MET:O	2.04	0.56
1:B:422:ALA:O	1:B:426:ARG:HG3	2.06	0.56
1:B:181:VAL:O	1:B:196:LEU:HD13	2.06	0.55
1:B:101:THR:HA	1:B:141:THR:CG2	2.36	0.55
1:A:397:ARG:HD2	1:A:400:GLU:OE1	2.07	0.55
1:A:232:VAL:HG11	1:B:195:ILE:HD12	1.89	0.55
1:B:214:ARG:O	1:B:218:THR:HG23	2.07	0.55
1:B:67:ASP:OD2	1:B:69:GLU:HB3	2.07	0.55
1:A:434:SER:HB3	1:A:437:GLU:HB2	1.88	0.54
1:B:173:LYS:HD3	2:B:659:HOH:O	2.07	0.54
1:A:409:ILE:HD13	1:A:435:ILE:HD11	1.88	0.54
1:B:232:VAL:HG13	1:B:357:GLU:HG3	1.89	0.54
1:A:446:THR:H	1:A:449:GLN:HE21	1.56	0.54
1:B:93:ASP:OD1	1:B:94:PRO:HD2	2.07	0.54
1:A:6:ARG:NH1	1:A:8:GLU:OE2	2.41	0.54
1:B:336:VAL:O	1:B:340:VAL:HG23	2.08	0.53
1:A:329:MET:HB2	1:A:330:PRO:HD3	1.89	0.53
1:B:408:ILE:HD11	1:B:454:LEU:HD11	1.91	0.53
1:B:292:ALA:O	1:B:296:ARG:HG3	2.08	0.53
1:B:130:SER:HB3	1:B:133:SER:HB2	1.90	0.53
1:B:412:ILE:HD12	1:B:435:ILE:HD13	1.90	0.53
1:A:142:ASN:O	1:A:146:PRO:HG3	2.08	0.53
1:A:167:MET:HB2	1:A:384:THR:HG21	1.91	0.53
1:A:232:VAL:HG13	1:A:357:GLU:HB3	1.91	0.53
1:A:54:LYS:HG3	1:A:75:VAL:HG13	1.90	0.53
1:A:23:TYR:HE2	1:A:28:ILE:HD11	1.73	0.53
1:A:202:GLU:O	1:A:206:ARG:HG3	2.09	0.52
1:A:199:GLN:HA	2:A:548:HOH:O	2.09	0.52
1:A:356:PHE:HB3	1:A:357:GLU:OE2	2.08	0.52
1:B:296:ARG:NH1	1:B:334:ASN:OD1	2.41	0.52
1:A:182:ILE:HG13	1:A:402:VAL:HG21	1.92	0.52
1:A:445:LEU:HD22	1:A:453:ILE:HD11	1.91	0.52
1:B:265:VAL:O	1:B:269:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:MET:CE	1:B:194:PRO:HG3	2.32	0.52
1:A:241:GLU:O	1:A:245:ILE:HG13	2.09	0.52
1:B:7:ILE:HA	1:B:15:LYS:O	2.09	0.52
1:B:269:GLN:HB3	1:B:357:GLU:HA	1.92	0.52
1:A:167:MET:HG3	1:A:384:THR:HG22	1.92	0.51
1:B:257:PRO:HB2	2:B:666:HOH:O	2.08	0.51
1:B:408:ILE:HD11	1:B:454:LEU:CD1	2.40	0.51
1:B:170:GLU:HG3	2:B:587:HOH:O	2.11	0.51
1:A:106:ASN:O	1:A:110:VAL:HG23	2.11	0.51
1:A:318:SER:OG	1:A:321:MET:HB3	2.11	0.51
1:A:440:ILE:HD11	1:A:447:GLU:OE1	2.11	0.51
1:B:336:VAL:CG2	1:B:379:VAL:HG11	2.34	0.51
1:A:73:TYR:CE1	1:A:119:MET:HB3	2.46	0.51
1:A:272:ASP:HA	2:A:525:HOH:O	2.10	0.51
1:B:464:ILE:HG12	1:B:465:ALA:N	2.23	0.50
1:B:80:GLU:HB3	1:B:86:TRP:HE1	1.75	0.50
1:A:157:LEU:O	1:A:161:ILE:HG13	2.12	0.50
1:A:12:LEU:HD12	1:A:29:ARG:CG	2.41	0.50
1:B:116:LEU:HG	1:B:129:ILE:HB	1.93	0.50
1:B:11:PHE:CE1	1:B:12:LEU:HG	2.46	0.50
1:A:170:GLU:OE1	1:A:389:LYS:HE2	2.12	0.50
1:B:99:ALA:HB2	1:B:360:VAL:CA	2.41	0.50
1:A:114:ARG:HD2	1:A:114:ARG:O	2.12	0.50
1:B:101:THR:CA	1:B:141:THR:HG21	2.41	0.50
1:B:263:HIS:CE1	1:B:265:VAL:HB	2.46	0.50
1:A:167:MET:HE3	1:A:380:PHE:HA	1.93	0.49
1:A:416:VAL:O	1:A:420:THR:HB	2.12	0.49
1:A:422:ALA:HB1	1:A:426:ARG:HH12	1.76	0.49
1:B:99:ALA:CB	1:B:360:VAL:HA	2.40	0.49
1:A:327:PRO:O	1:A:330:PRO:HD2	2.13	0.49
1:A:330:PRO:O	1:A:333:MET:HB3	2.11	0.49
1:B:176:ASP:HA	1:B:179:ALA:HB2	1.95	0.49
1:A:296:ARG:HD2	1:A:331:GLU:HG2	1.95	0.49
1:B:199:GLN:NE2	1:B:460:ILE:HD12	2.27	0.48
1:B:167:MET:CB	1:B:384:THR:HG21	2.43	0.48
1:A:12:LEU:HD12	1:A:29:ARG:HG3	1.95	0.48
1:B:225:ILE:HG12	1:B:259:ARG:O	2.14	0.48
1:A:287:ASN:OD1	1:B:272:ASP:HB3	2.14	0.48
1:B:51:ILE:CA	1:B:82:ILE:HD11	2.42	0.48
1:A:73:TYR:CD1	1:A:119:MET:HB3	2.49	0.48
1:A:263:HIS:HB3	1:A:266:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:HG13	1:B:357:GLU:CB	2.43	0.48
1:A:408:ILE:O	1:A:408:ILE:HG12	2.12	0.48
1:B:416:VAL:O	1:B:416:VAL:HG12	2.13	0.48
1:B:464:ILE:HG23	1:B:466:GLY:H	1.79	0.48
1:B:134:HIS:HA	1:B:137:MET:HE3	1.94	0.48
1:A:236:LEU:O	1:A:237:ASN:HB2	2.13	0.48
1:B:204:TYR:O	1:B:208:ILE:HG13	2.13	0.48
1:A:223:TYR:CE2	1:A:257:PRO:HD2	2.49	0.48
1:B:26:GLN:HE22	1:B:105:MET:HG3	1.79	0.47
1:B:362:GLU:N	1:B:363:PRO:HD2	2.28	0.47
1:A:345:LEU:HD23	1:A:345:LEU:O	2.14	0.47
1:B:8:GLU:HB2	1:B:25:VAL:CG1	2.42	0.47
1:B:369:LEU:O	1:B:373:ILE:HG13	2.14	0.47
1:A:71:GLY:O	1:A:75:VAL:HG23	2.13	0.47
1:A:153:VAL:O	1:A:157:LEU:HB2	2.14	0.47
1:B:242:TYR:O	1:B:246:VAL:HG12	2.14	0.47
1:A:196:LEU:HD23	1:A:460:ILE:HG21	1.97	0.47
1:A:462:PRO:HA	1:B:235:GLY:O	2.15	0.47
1:B:225:ILE:HD11	1:B:247:THR:HG23	1.96	0.47
1:B:228:GLY:HA3	1:B:243:ILE:HG12	1.96	0.47
1:A:315:GLN:HE21	1:A:315:GLN:HA	1.79	0.47
1:A:136:ASN:O	1:A:139:GLN:HG2	2.15	0.47
1:A:195:ILE:HD12	1:B:232:VAL:CG1	2.45	0.47
1:B:156:LEU:CD1	1:B:370:ILE:HG23	2.45	0.47
1:A:220:ASN:HA	1:A:223:TYR:CD1	2.50	0.47
1:B:457:TYR:O	1:B:460:ILE:HG13	2.15	0.46
1:A:239:ASP:O	1:A:242:TYR:HB3	2.16	0.46
1:B:196:LEU:HG	1:B:460:ILE:CD1	2.43	0.46
1:A:8:GLU:HB3	1:A:25:VAL:HG13	1.98	0.46
1:B:204:TYR:O	1:B:207:VAL:HG12	2.16	0.46
1:B:26:GLN:HE21	1:B:26:GLN:HB3	1.62	0.46
1:A:6:ARG:HG2	1:A:7:ILE:N	2.30	0.46
1:B:306:LEU:N	1:B:306:LEU:HD23	2.30	0.46
1:A:457:TYR:O	1:A:460:ILE:HG13	2.16	0.46
1:B:49:LEU:HD13	1:B:148:ALA:HB1	1.97	0.46
1:B:53:LYS:HG3	1:B:111:ILE:HD12	1.97	0.46
1:B:327:PRO:O	1:B:331:GLU:HG3	2.16	0.45
1:A:167:MET:HE1	1:A:380:PHE:HA	1.98	0.45
1:A:318:SER:HB3	1:A:321:MET:HB3	1.99	0.45
1:A:329:MET:O	1:A:332:VAL:HG12	2.16	0.45
1:B:200:GLU:O	1:B:203:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:THR:O	1:B:188:HIS:CB	2.63	0.45
1:A:445:LEU:HB2	1:A:450:LEU:HD13	1.99	0.45
1:B:357:GLU:N	1:B:357:GLU:CD	2.70	0.45
1:B:357:GLU:CD	1:B:357:GLU:H	2.18	0.45
1:B:53:LYS:HD2	1:B:135:VAL:HG12	1.99	0.45
1:A:203:ALA:HA	1:B:266:ASP:HB2	1.99	0.45
1:A:196:LEU:CB	1:A:460:ILE:HD13	2.41	0.45
1:A:195:ILE:HD11	1:B:265:VAL:HG11	1.99	0.45
1:A:243:ILE:O	1:A:246:VAL:HG12	2.16	0.45
1:A:187:THR:HB	1:B:358:LEU:HD23	1.97	0.45
1:B:39:TYR:O	1:B:94:PRO:HD3	2.17	0.45
1:B:62:GLU:OE2	1:B:245:ILE:HD13	2.17	0.45
1:A:315:GLN:HE21	1:A:315:GLN:CA	2.30	0.44
1:A:237:ASN:OD1	1:B:414:PRO:HG2	2.17	0.44
1:A:36:ILE:N	1:A:36:ILE:HD13	2.32	0.44
1:B:383:PHE:O	1:B:387:CYS:HB3	2.17	0.44
1:B:337:ALA:O	1:B:341:PHE:CD1	2.71	0.44
1:B:384:THR:HA	1:B:388:LEU:HB3	1.99	0.44
1:A:145:PHE:N	1:A:146:PRO:HD2	2.32	0.44
1:B:229:ALA:HA	1:B:264:LEU:HD23	2.00	0.44
1:B:413:ASN:HB3	1:B:414:PRO:HD3	1.99	0.44
1:B:153:VAL:CG1	1:B:222:LEU:HD21	2.48	0.43
1:B:285:MET:HB3	1:B:337:ALA:HA	2.00	0.43
1:A:204:TYR:O	1:A:207:VAL:HG12	2.17	0.43
1:B:141:THR:HG22	1:B:141:THR:O	2.18	0.43
1:B:208:ILE:O	1:B:211:ASP:HB2	2.18	0.43
1:A:430:LEU:N	1:A:430:LEU:HD22	2.33	0.43
1:A:188:HIS:O	1:A:189:LEU:HB2	2.18	0.43
1:B:321:MET:SD	1:B:324:LYS:HD2	2.58	0.43
1:A:196:LEU:HB2	1:A:199:GLN:HG3	2.00	0.43
1:A:119:MET:CE	1:A:129:ILE:HD11	2.49	0.43
1:B:197:LEU:HD22	1:B:201:PHE:CD2	2.54	0.43
1:B:411:ALA:O	1:B:414:PRO:HD2	2.18	0.43
1:B:145:PHE:N	1:B:146:PRO:HD2	2.34	0.43
1:B:343:ASN:ND2	1:B:371:GLN:HE21	2.14	0.43
1:B:365:LEU:HD23	1:B:365:LEU:C	2.40	0.43
1:B:179:ALA:O	1:B:196:LEU:HD12	2.19	0.43
1:B:343:ASN:HB3	1:B:368:ASN:HB3	2.00	0.42
1:A:318:SER:HB3	1:A:321:MET:O	2.19	0.42
1:B:8:GLU:OE1	1:B:25:VAL:HG22	2.19	0.42
1:A:49:LEU:O	1:A:53:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ILE:O	1:B:32:GLU:HG3	2.19	0.42
1:A:435:ILE:HG22	2:A:708:HOH:O	2.19	0.42
1:A:167:MET:HG3	1:A:384:THR:CG2	2.49	0.42
1:A:343:ASN:CG	1:A:368:ASN:HD22	2.23	0.42
1:A:385:GLU:OE1	1:A:389:LYS:HD2	2.19	0.42
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.87	0.42
1:A:208:ILE:O	1:A:212:ILE:HG13	2.20	0.42
1:A:18:PRO:HB2	1:A:21:ALA:HB2	2.02	0.42
1:A:157:LEU:HD23	1:A:219:ARG:HG2	2.02	0.42
1:B:63:VAL:HG12	1:B:63:VAL:O	2.19	0.42
1:B:263:HIS:HE1	1:B:265:VAL:HB	1.82	0.42
1:B:318:SER:HB2	1:B:321:MET:HB2	2.00	0.42
1:A:189:LEU:HG	1:B:355:GLN:NE2	2.35	0.42
1:A:408:ILE:HG23	1:A:435:ILE:HG21	2.00	0.41
1:B:53:LYS:HD3	1:B:53:LYS:HA	1.79	0.41
1:A:112:ALA:HB2	1:A:135:VAL:HG21	2.02	0.41
1:B:45:LEU:HD22	1:B:49:LEU:HD22	2.03	0.41
1:B:453:ILE:C	1:B:455:ASN:H	2.23	0.41
1:A:232:VAL:HG13	1:A:357:GLU:CB	2.50	0.41
1:A:78:ALA:O	1:A:82:ILE:HG13	2.21	0.41
1:A:371:GLN:O	1:A:375:ILE:HG23	2.21	0.41
1:A:383:PHE:O	1:A:387:CYS:HB3	2.21	0.41
1:A:348:THR:HG23	1:B:286:ILE:HD11	2.03	0.41
1:A:352:GLU:HG3	2:A:526:HOH:O	2.21	0.41
1:A:168:GLN:NE2	1:A:205:ALA:HB1	2.35	0.41
1:A:10:ASP:C	1:A:12:LEU:H	2.24	0.41
1:B:409:ILE:HG23	1:B:410:THR:N	2.35	0.41
1:A:40:ARG:HG3	1:A:40:ARG:HH11	1.86	0.41
1:A:143:ASP:OD2	1:A:144:ALA:N	2.53	0.41
1:A:167:MET:CB	1:A:384:THR:HG21	2.51	0.41
1:A:45:LEU:O	1:A:49:LEU:HD22	2.21	0.40
1:A:105:MET:O	1:A:109:GLU:HG3	2.21	0.40
1:B:54:LYS:HD2	1:B:79:ASP:OD2	2.22	0.40
1:B:184:MET:HA	1:B:184:MET:HE2	2.02	0.40
1:A:405:SER:O	1:A:408:ILE:HG22	2.20	0.40
1:A:166:TYR:OH	1:A:389:LYS:NZ	2.47	0.40
1:A:328:VAL:HG23	1:A:329:MET:N	2.36	0.40
1:A:10:ASP:C	1:A:12:LEU:N	2.75	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:709:HOH:O	2:B:713:HOH:O[2_555]	0.16	2.04
2:B:594:HOH:O	2:B:594:HOH:O[2_555]	1.03	1.17

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	460/468 (98%)	422 (92%)	33 (7%)	5 (1%)	17	31
1	B	460/468 (98%)	424 (92%)	30 (6%)	6 (1%)	15	26
All	All	920/936 (98%)	846 (92%)	63 (7%)	11 (1%)	16	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA
1	A	417	GLY
1	A	444	VAL
1	B	230	THR
1	B	443	GLY
1	A	442	TYR
1	B	120	GLY
1	B	387	CYS
1	B	464	ILE
1	B	444	VAL
1	A	302	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	374/394 (95%)	351 (94%)	23 (6%)	23 42
1	B	376/394 (95%)	350 (93%)	26 (7%)	19 35
All	All	750/788 (95%)	701 (94%)	49 (6%)	21 39

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	45	LEU
1	A	49	LEU
1	A	72	GLN
1	A	106	ASN
1	A	125	ASN
1	A	132	ASN
1	A	159	GLN
1	A	170	GLU
1	A	190	GLN
1	A	196	LEU
1	A	197	LEU
1	A	266	ASP
1	A	295	LEU
1	A	306	LEU
1	A	307	SER
1	A	315	GLN
1	A	352	GLU
1	A	357	GLU
1	A	369	LEU
1	A	385	GLU
1	A	442	TYR
1	A	444	VAL
1	B	25	VAL
1	B	29	ARG
1	B	31	THR
1	B	45	LEU
1	B	49	LEU
1	B	58	LEU
1	B	106	ASN
1	B	132	ASN
1	B	157	LEU
1	B	190	GLN
1	B	196	LEU

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Mol	Chain	Res	Type
1	B	197	LEU
1	B	230	THR
1	B	244	SER
1	B	266	ASP
1	B	306	LEU
1	B	307	SER
1	B	315	GLN
1	B	325	VAL
1	B	345	LEU
1	B	352	GLU
1	B	357	GLU
1	B	369	LEU
1	B	401	TYR
1	B	442	TYR
1	B	447	GLU

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	96	GLN
1	A	125	ASN
1	A	132	ASN
1	A	190	GLN
1	A	217	ASN
1	A	221	ASN
1	A	269	GLN
1	A	315	GLN
1	A	355	GLN
1	A	368	ASN
1	A	371	GLN
1	A	449	GLN
1	A	451	ASN
1	B	26	GLN
1	B	96	GLN
1	B	125	ASN
1	B	132	ASN
1	B	190	GLN
1	B	217	ASN
1	B	343	ASN
1	B	355	GLN
1	B	368	ASN
1	B	371	GLN

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Mol	Chain	Res	Type
1	B	449	GLN
1	B	461	HIS

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	462/468 (98%)	0.08	25 (5%)	29	33	13, 29, 90, 101	0
1	B	462/468 (98%)	0.17	17 (3%)	45	50	16, 41, 76, 89	0
All	All	924/936 (98%)	0.12	42 (4%)	37	42	13, 33, 84, 101	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	ILE	9.7
1	A	464	ILE	7.6
1	A	319	SER	5.7
1	A	432	GLY	5.5
1	B	320	ILE	5.0
1	B	9	LYS	4.2
1	A	465	ALA	4.2
1	A	448	GLU	4.1
1	A	463	GLY	4.1
1	A	466	GLY	4.1
1	B	464	ILE	3.8
1	A	317	GLY	3.7
1	A	409	ILE	3.5
1	A	424	LEU	3.5
1	B	450	LEU	3.4
1	B	321	MET	3.4
1	A	435	ILE	3.2
1	A	453	ILE	3.0
1	B	118	LEU	2.9
1	B	319	SER	2.9
1	A	442	TYR	2.8
1	A	457	TYR	2.8
1	B	72	GLN	2.7
1	B	13	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	440	ILE	2.6
1	A	451	ASN	2.5
1	A	13	GLY	2.5
1	A	434	SER	2.5
1	A	439	CYS	2.5
1	A	446	THR	2.4
1	B	64	GLY	2.4
1	A	447	GLU	2.4
1	B	120	GLY	2.3
1	A	449	GLN	2.3
1	B	73	TYR	2.3
1	B	463	GLY	2.2
1	A	438	LEU	2.2
1	B	466	GLY	2.1
1	B	119	MET	2.1
1	A	445	LEU	2.1
1	B	63	VAL	2.0
1	B	6	ARG	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.