WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:35 PM GMT

|		
PDB ID	:	1GCJ
Title	:	N-TERMINAL FRAGMENT OF IMPORTIN-BETA
Authors	:	Lee, S.J.; Imamoto, N.; Sakai, H.; Nakagawa, A.; Kose, S.; Koike, M.; Yamamoto, M.; Kumasaka, T.; Yoneda, Y.; Tsukihara, T.
Deposited on	:	2000-07-31
Resolution	:	2.60 Å(reported)

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 2.60 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.
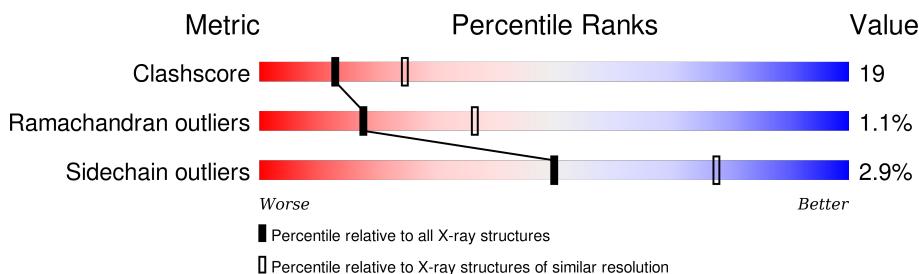
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	460	65% 　　　 33% 　 •
1	B	460	67% 　　　 31% 　 •
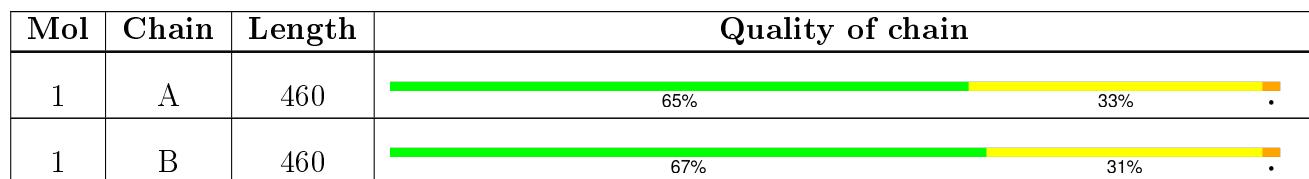
2   Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7389 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 IMPORTIN BETA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	460	Total 3589	C 2260	N 597	O 708	S 11	Se 13	0	0	0
1	B	460	Total 3589	C 2260	N 597	O 708	S 11	Se 13	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	146	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	181	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	219	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	245	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	252	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	256	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	268	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	291	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	353	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	388	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	410	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	417	MSE	MET	MODIFIED RESIDUE	UNP P70168
A	450	VAL	-	CLONING ARTIFACT	UNP P70168
A	451	PRO	-	CLONING ARTIFACT	UNP P70168
A	452	ASN	-	CLONING ARTIFACT	UNP P70168
A	453	SER	-	CLONING ARTIFACT	UNP P70168
A	454	SER	-	CLONING ARTIFACT	UNP P70168
A	500	PRO	-	CLONING ARTIFACT	UNP P70168
A	501	ASP	-	CLONING ARTIFACT	UNP P70168
A	502	TYR	-	CLONING ARTIFACT	UNP P70168
A	503	ALA	-	CLONING ARTIFACT	UNP P70168
A	504	SER	-	CLONING ARTIFACT	UNP P70168
A	505	GLY	-	CLONING ARTIFACT	UNP P70168
B	1	MSE	MET	MODIFIED RESIDUE	UNP P70168

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Chain	Residue	Modelled	Actual	Comment	Reference
B	146	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	181	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	219	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	245	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	252	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	256	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	268	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	291	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	353	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	388	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	410	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	417	MSE	MET	MODIFIED RESIDUE	UNP P70168
B	450	VAL	-	CLONING ARTIFACT	UNP P70168
B	451	PRO	-	CLONING ARTIFACT	UNP P70168
B	452	ASN	-	CLONING ARTIFACT	UNP P70168
B	453	SER	-	CLONING ARTIFACT	UNP P70168
B	454	SER	-	CLONING ARTIFACT	UNP P70168
B	500	PRO	-	CLONING ARTIFACT	UNP P70168
B	501	ASP	-	CLONING ARTIFACT	UNP P70168
B	502	TYR	-	CLONING ARTIFACT	UNP P70168
B	503	ALA	-	CLONING ARTIFACT	UNP P70168
B	504	SER	-	CLONING ARTIFACT	UNP P70168
B	505	GLY	-	CLONING ARTIFACT	UNP P70168

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	115	Total O 115 115	0	0
2	B	96	Total O 96 96	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.

Note EDS was not executed.

- Molecule 1: IMPORTIN BETA

Chain A:

- Molecule 1: IMPORTIN BETA

Chain B:
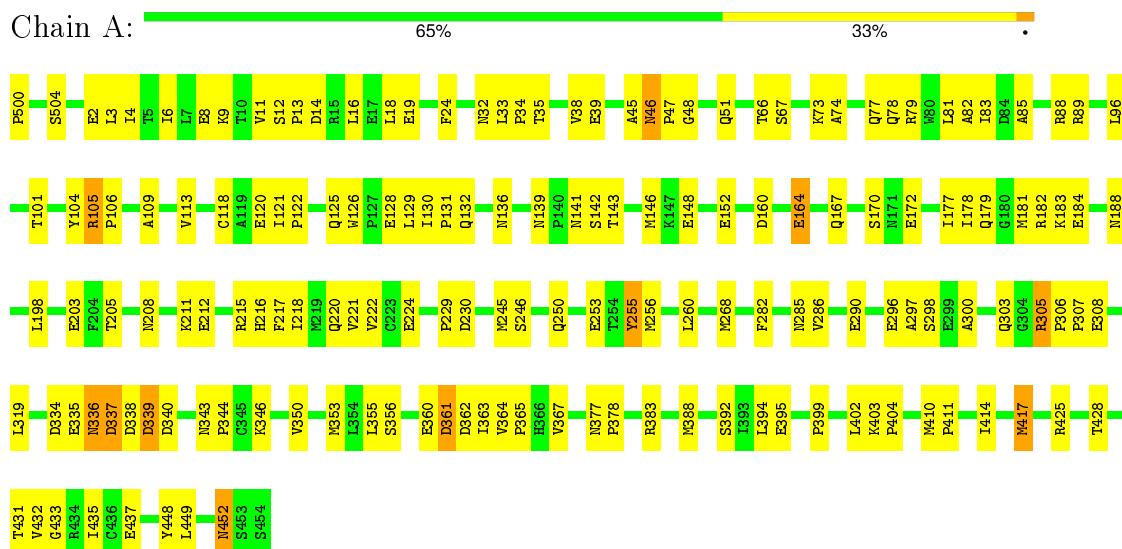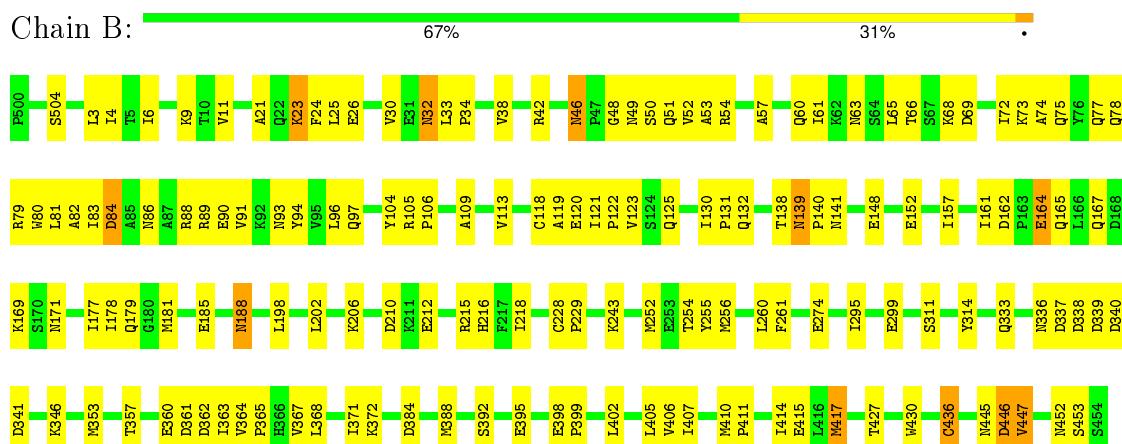
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.83Å 103.78Å 126.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.18 – 2.60	Depositor
% Data completeness (in resolution range)	97.9 (39.18-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7389	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

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	0.33	0/3643	0.56	0/4938
1	B	0.35	1/3643 (0.0%)	0.54	0/4938
All	All	0.34	1/7286 (0.0%)	0.55	0/9876

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	436	CYS	CB-SG	6.80	1.93	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3589	0	3563	140	0
1	B	3589	0	3563	141	0
2	A	115	0	0	15	0
2	B	96	0	0	7	0
All	All	7389	0	7126	275	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 19.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HB3	1:A:106:PRO:HD3	1.44	0.99
1:B:105:ARG:HB3	1:B:106:PRO:HD3	1.45	0.98
1:B:188:ASN:HD22	1:B:188:ASN:H	1.12	0.95
1:A:170:SER:HB2	1:A:208:ASN:HD21	1.30	0.94
1:A:177:ILE:HG22	1:A:181:MSE:HE2	1.56	0.88
1:B:256:MSE:HE3	1:B:261:PHE:HB2	1.60	0.84
1:B:42:ARG:HG2	1:B:94:TYR:CE1	2.13	0.84
1:B:157:ILE:HG23	1:B:161:ILE:HD12	1.61	0.81
1:B:23:LYS:HE2	1:B:23:LYS:HA	1.63	0.80
1:B:46:ASN:HB3	1:B:49:ASN:HD22	1.48	0.78
1:B:65:LEU:HG	2:B:553:HOH:O	1.82	0.78
1:B:188:ASN:ND2	1:B:188:ASN:H	1.82	0.78
1:B:120:GLU:HB3	1:B:125:GLN:HB2	1.68	0.75
1:A:46:ASN:ND2	1:A:48:GLY:H	1.84	0.75
1:B:452:ASN:ND2	1:B:453:SER:H	1.84	0.74
1:B:93:ASN:O	1:B:97:GLN:HG2	1.88	0.74
1:B:177:ILE:HG22	1:B:181:MSE:HE2	1.69	0.74
1:A:143:THR:HG23	1:A:146:MSE:H	1.53	0.74
1:B:181:MSE:HE1	1:B:198:LEU:HD22	1.67	0.73
1:B:360:GLU:O	1:B:363:ILE:HG22	1.88	0.73
1:A:449:LEU:HB3	1:B:447:VAL:HG21	1.70	0.73
1:A:181:MSE:HE1	1:A:198:LEU:HD22	1.68	0.73
1:B:88:ARG:HH22	1:B:125:GLN:HE21	1.34	0.72
1:A:364:VAL:HB	1:A:365:PRO:HD3	1.72	0.72
1:A:81:LEU:HA	1:A:88:ARG:NH1	2.04	0.72
1:B:130:ILE:HG13	1:B:169:LYS:HD3	1.70	0.72
1:A:361:ASP:HB3	2:A:616:HOH:O	1.88	0.72
1:B:46:ASN:HB3	1:B:49:ASN:ND2	2.04	0.71
1:B:77:GLN:O	1:B:81:LEU:HD13	1.91	0.70
1:A:81:LEU:HA	1:A:88:ARG:HH11	1.56	0.70
1:A:208:ASN:HA	1:A:211:LYS:HE2	1.74	0.69
1:B:38:VAL:O	1:B:42:ARG:HG3	1.93	0.69
1:B:73:LYS:O	1:B:77:GLN:HG3	1.92	0.69
1:A:300:ALA:HA	1:A:303:GLN:HE21	1.56	0.69
1:A:337:ASP:CG	1:A:340:ASP:H	1.96	0.69
1:A:297:ALA:HA	1:A:307:PRO:HG3	1.73	0.69
1:A:297:ALA:HA	1:A:307:PRO:CG	2.23	0.68
1:B:139:ASN:HD22	1:B:140:PRO:N	1.91	0.68
1:A:253:GLU:HB3	2:A:527:HOH:O	1.93	0.68
1:B:162:ASP:HB3	1:B:165:GLN:HG2	1.76	0.67
1:A:177:ILE:CG2	1:A:181:MSE:HE2	2.24	0.67
1:A:216:HIS:HB2	2:A:589:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:HD13	1:B:417:MSE:HE1	1.76	0.67
1:B:148:GLU:O	1:B:152:GLU:HG3	1.94	0.67
1:A:45:ALA:O	1:A:47:PRO:HD3	1.94	0.67
1:B:339:ASP:HA	1:B:346:LYS:NZ	2.09	0.66
1:B:88:ARG:HH22	1:B:125:GLN:NE2	1.94	0.66
1:B:86:ASN:HA	1:B:89:ARG:NH1	2.10	0.66
1:B:139:ASN:ND2	1:B:141:ASN:H	1.94	0.65
1:A:105:ARG:CB	1:A:106:PRO:HD3	2.24	0.64
1:B:388:MSE:HE3	1:B:392:SER:OG	1.98	0.64
1:B:164:GLU:HA	1:B:167:GLN:HE21	1.63	0.64
1:A:388:MSE:HE3	1:A:392:SER:OG	1.97	0.64
1:B:452:ASN:ND2	1:B:453:SER:N	2.46	0.64
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.79	0.63
1:B:139:ASN:HD22	1:B:139:ASN:C	2.02	0.63
1:A:51:GLN:OE1	1:A:104:TYR:HB3	1.99	0.63
1:B:34:PRO:HG3	1:B:83:ILE:HG12	1.79	0.62
1:A:4:ILE:O	1:A:8:GLU:HG3	1.98	0.62
1:B:72:ILE:HA	1:B:75:GLN:HE21	1.63	0.62
1:A:148:GLU:O	1:A:152:GLU:HG3	1.98	0.62
1:B:177:ILE:HG22	1:B:181:MSE:CE	2.29	0.62
1:A:177:ILE:HG22	1:A:181:MSE:CE	2.28	0.62
1:A:256:MSE:HA	1:A:260:LEU:HB2	1.82	0.62
1:A:85:ALA:O	1:A:89:ARG:HG3	2.00	0.62
1:A:6:ILE:HG21	1:A:24:PHE:HD2	1.64	0.61
1:B:362:ASP:O	1:B:365:PRO:HD2	2.01	0.61
1:B:109:ALA:O	1:B:113:VAL:HG23	2.00	0.61
1:A:245:MSE:HE3	1:A:282:PHE:CZ	2.36	0.60
1:B:256:MSE:CE	1:B:261:PHE:HB2	2.29	0.60
1:A:203:GLU:HB2	2:A:582:HOH:O	2.00	0.60
1:A:126:TRP:HD1	1:A:128:GLU:OE2	1.84	0.60
1:B:32:ASN:ND2	1:B:34:PRO:HD2	2.16	0.60
1:A:286:VAL:O	1:A:290:GLU:HG3	2.02	0.60
1:A:449:LEU:HD13	1:B:417:MSE:CE	2.31	0.59
1:B:177:ILE:CG2	1:B:181:MSE:HE2	2.32	0.59
1:B:130:ILE:HB	1:B:131:PRO:HD3	1.85	0.59
2:A:603:HOH:O	1:B:68:LYS:HE2	2.02	0.59
1:B:60:GLN:HG2	2:B:552:HOH:O	2.03	0.58
1:A:220:GLN:O	1:A:224:GLU:HG3	2.03	0.58
1:B:407:ILE:HG23	1:B:446:ASP:OD2	2.03	0.58
1:A:337:ASP:C	1:A:339:ASP:H	2.06	0.58
1:B:446:ASP:O	1:B:447:VAL:HB	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HB2	1:A:306:PRO:HD2	1.86	0.57
1:B:339:ASP:HA	1:B:346:LYS:HZ3	1.67	0.57
1:B:96:LEU:HD13	1:B:132:GLN:HG2	1.86	0.57
1:A:11:VAL:O	1:A:11:VAL:HG12	2.04	0.57
1:A:346:LYS:HB2	1:A:346:LYS:NZ	2.19	0.57
1:A:362:ASP:O	1:A:365:PRO:HD2	2.05	0.57
1:B:252:MSE:HE3	1:B:260:LEU:CD1	2.34	0.56
1:A:188:ASN:ND2	1:A:230:ASP:HB2	2.20	0.56
1:A:417:MSE:HA	1:A:417:MSE:HE3	1.88	0.56
1:B:410:MSE:HB3	1:B:411:PRO:HD3	1.86	0.56
1:B:139:ASN:HD22	1:B:140:PRO:CD	2.18	0.56
1:A:338:ASP:O	1:A:339:ASP:HB2	2.06	0.56
1:A:66:THR:HG22	1:A:67:SER:N	2.21	0.56
1:B:398:GLU:OE2	1:B:399:PRO:HD2	2.06	0.56
1:A:73:LYS:O	1:A:77:GLN:HG3	2.06	0.56
1:A:433:GLY:O	1:A:437:GLU:HB2	2.06	0.56
1:A:33:LEU:HB3	1:A:34:PRO:HD3	1.87	0.56
1:B:357:THR:HG22	1:B:395:GLU:HG2	1.87	0.55
1:A:164:GLU:HA	1:A:167:GLN:HE21	1.71	0.55
1:B:162:ASP:OD2	1:B:164:GLU:HG2	2.07	0.55
1:B:364:VAL:HB	1:B:365:PRO:HD3	1.89	0.55
1:A:452:ASN:HB2	1:B:445:ASN:O	2.05	0.55
1:A:51:GLN:HG3	1:A:104:TYR:CD2	2.42	0.55
1:A:126:TRP:CE3	1:A:129:LEU:HD22	2.42	0.55
1:B:452:ASN:HD22	1:B:453:SER:N	2.06	0.54
1:A:350:VAL:HA	1:A:353:MSE:HE3	1.89	0.54
1:B:105:ARG:CB	1:B:106:PRO:HD3	2.28	0.54
1:B:72:ILE:O	1:B:75:GLN:HG2	2.07	0.54
1:A:346:LYS:O	1:A:350:VAL:HG23	2.08	0.54
1:B:11:VAL:O	1:B:11:VAL:HG12	2.07	0.54
1:A:303:GLN:HG3	1:A:305:ARG:HG2	1.88	0.54
1:B:33:LEU:HB3	1:B:34:PRO:HD3	1.88	0.54
1:B:181:MSE:CE	1:B:198:LEU:HB2	2.37	0.54
1:A:336:ASN:O	1:A:337:ASP:O	2.26	0.53
1:A:128:GLU:CD	1:A:128:GLU:H	2.11	0.53
1:A:128:GLU:HB2	2:A:574:HOH:O	2.07	0.53
1:B:252:MSE:HE3	1:B:260:LEU:HD13	1.91	0.53
1:A:428:THR:O	1:A:432:VAL:HG23	2.09	0.53
1:A:178:ILE:HG23	1:A:221:VAL:HG21	1.90	0.53
1:A:410:MSE:HB3	1:A:411:PRO:HD3	1.91	0.53
1:A:403:LYS:N	1:A:404:PRO:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:O	1:A:336:ASN:N	2.40	0.52
1:B:256:MSE:HE3	1:B:261:PHE:CB	2.36	0.52
1:B:105:ARG:HB3	1:B:106:PRO:CD	2.30	0.52
1:A:164:GLU:H	1:A:164:GLU:CD	2.13	0.52
1:B:164:GLU:HA	1:B:167:GLN:NE2	2.25	0.52
1:A:183:LYS:HD3	1:A:224:GLU:OE2	2.10	0.52
1:B:202:LEU:HD12	1:B:243:LYS:HD3	1.90	0.52
1:A:360:GLU:O	1:A:363:ILE:HG22	2.10	0.52
1:B:32:ASN:HD22	1:B:34:PRO:HD2	1.74	0.51
1:B:46:ASN:ND2	1:B:48:GLY:H	2.08	0.51
1:A:297:ALA:HB3	2:A:600:HOH:O	2.09	0.51
1:B:57:ALA:O	1:B:61:ILE:HG13	2.09	0.51
1:B:139:ASN:ND2	1:B:139:ASN:C	2.63	0.51
1:A:14:ASP:OD1	1:A:16:LEU:N	2.43	0.51
1:A:300:ALA:O	1:A:303:GLN:HG2	2.11	0.51
1:B:216:HIS:HE1	1:B:254:THR:HG21	1.75	0.51
1:A:395:GLU:HB3	2:A:542:HOH:O	2.10	0.51
1:A:136:ASN:ND2	1:A:146:MSE:SE	2.94	0.51
1:B:141:ASN:N	1:B:141:ASN:HD22	2.08	0.50
1:A:34:PRO:HG3	1:A:83:ILE:HG12	1.93	0.50
1:B:256:MSE:HA	1:B:260:LEU:HB2	1.92	0.50
1:A:300:ALA:HA	1:A:303:GLN:NE2	2.25	0.50
1:B:336:ASN:CG	1:B:337:ASP:H	2.15	0.50
1:A:136:ASN:HD22	1:A:146:MSE:SE	2.44	0.50
1:B:74:ALA:O	1:B:78:GLN:HG2	2.12	0.50
1:A:417:MSE:O	1:A:425:ARG:HG2	2.12	0.49
1:B:181:MSE:HE1	1:B:198:LEU:HD13	1.94	0.49
1:A:120:GLU:HB3	1:A:125:GLN:HB2	1.93	0.49
1:A:170:SER:HB2	1:A:208:ASN:ND2	2.12	0.49
1:B:66:THR:HG22	1:B:73:LYS:NZ	2.27	0.49
1:A:305:ARG:HA	2:A:603:HOH:O	2.12	0.49
1:B:402:LEU:HA	1:B:405:LEU:HD12	1.93	0.49
1:B:4:ILE:HD13	1:B:49:ASN:OD1	2.12	0.49
1:B:341:ASP:O	1:B:346:LYS:HD2	2.12	0.49
1:A:363:ILE:O	1:A:367:VAL:HG23	2.12	0.49
1:A:18:LEU:HD23	1:A:18:LEU:O	2.12	0.49
1:A:205:THR:HG22	1:A:208:ASN:ND2	2.27	0.49
1:B:84:ASP:OD2	1:B:86:ASN:HB2	2.12	0.48
1:B:162:ASP:CG	1:B:164:GLU:HG2	2.34	0.48
1:B:130:ILE:HG13	1:B:169:LYS:CD	2.41	0.48
1:B:86:ASN:HA	1:B:89:ARG:HH12	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HA	2:A:579:HOH:O	2.14	0.48
1:A:132:GLN:O	1:A:136:ASN:OD1	2.32	0.48
1:B:50:SER:O	1:B:54:ARG:HG3	2.14	0.48
1:B:274:GLU:HG3	2:B:524:HOH:O	2.13	0.48
1:A:96:LEU:HD13	1:A:132:GLN:HG2	1.96	0.48
1:B:79:ARG:O	1:B:82:ALA:HB3	2.14	0.47
1:A:105:ARG:NH2	2:A:520:HOH:O	2.38	0.47
1:B:80:TRP:HD1	1:B:81:LEU:HD12	1.77	0.47
1:B:215:ARG:HD2	1:B:255:TYR:OH	2.14	0.47
1:B:256:MSE:HG2	1:B:314:TYR:CD2	2.50	0.47
1:B:34:PRO:O	1:B:38:VAL:HG23	2.14	0.47
1:B:52:VAL:HG23	1:B:53:ALA:N	2.29	0.47
1:B:21:ALA:O	1:B:25:LEU:HG	2.14	0.47
1:A:361:ASP:N	1:A:361:ASP:OD1	2.48	0.47
1:A:305:ARG:HH11	1:A:305:ARG:HG2	1.80	0.47
1:A:218:ILE:O	1:A:222:VAL:HG23	2.15	0.47
1:B:63:ASN:HD22	1:B:63:ASN:N	2.13	0.46
1:A:449:LEU:CB	1:B:447:VAL:HG21	2.42	0.46
1:A:343:ASN:HB2	1:A:344:PRO:HD2	1.97	0.46
1:B:6:ILE:HD13	1:B:24:PHE:CD2	2.49	0.46
1:A:128:GLU:CD	1:A:128:GLU:N	2.68	0.46
1:A:9:LYS:C	1:A:11:VAL:H	2.18	0.46
1:A:105:ARG:HB3	1:A:106:PRO:CD	2.29	0.46
1:A:32:ASN:ND2	1:A:35:THR:HB	2.31	0.46
1:A:34:PRO:O	1:A:38:VAL:HG23	2.16	0.46
1:B:23:LYS:HA	1:B:23:LYS:CE	2.42	0.45
1:A:250:GLN:HB2	2:A:588:HOH:O	2.17	0.45
1:A:46:ASN:HD22	1:A:46:ASN:C	2.19	0.45
1:B:295:ILE:O	1:B:299:GLU:HG3	2.16	0.45
1:B:178:ILE:HD11	1:B:218:ILE:HG12	1.98	0.45
1:B:38:VAL:HG13	1:B:90:GLU:HG2	1.99	0.45
1:A:6:ILE:HG21	1:A:24:PHE:CD2	2.48	0.45
1:A:346:LYS:HZ2	1:A:346:LYS:HB2	1.78	0.45
1:A:66:THR:HG22	1:A:67:SER:H	1.81	0.45
1:A:106:PRO:HD3	2:A:571:HOH:O	2.16	0.44
1:B:372:LYS:HD3	1:B:372:LYS:HA	1.65	0.44
1:A:448:TYR:CD1	1:B:452:ASN:HA	2.52	0.44
1:A:164:GLU:CD	1:A:164:GLU:N	2.70	0.44
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.18	0.44
1:A:296:GLU:OE2	1:A:308:GLU:HG3	2.17	0.44
1:B:83:ILE:HG23	2:B:558:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLN:NE2	1:B:384:ASP:OD1	2.51	0.44
1:A:246:SER:HB3	1:A:285:ASN:ND2	2.32	0.44
1:A:179:GLN:NE2	1:A:182:ARG:HD2	2.33	0.44
1:A:500:PRO:HB2	1:A:39:GLU:OE2	2.17	0.44
1:B:34:PRO:HG3	1:B:83:ILE:CG1	2.46	0.44
1:B:121:ILE:HB	1:B:122:PRO:HD3	1.99	0.44
1:A:205:THR:HG22	1:A:208:ASN:HD22	1.83	0.44
1:B:338:ASP:C	1:B:340:ASP:H	2.22	0.43
1:B:256:MSE:HG2	1:B:314:TYR:CE2	2.54	0.43
1:B:9:LYS:C	1:B:11:VAL:H	2.21	0.43
1:A:79:ARG:O	1:A:82:ALA:HB3	2.18	0.43
1:B:81:LEU:CD1	1:B:119:ALA:HB1	2.49	0.43
1:B:181:MSE:HE1	1:B:198:LEU:HB2	1.99	0.43
1:B:171:ASN:HD22	1:B:171:ASN:N	2.16	0.43
1:A:121:ILE:N	1:A:122:PRO:CD	2.82	0.43
1:B:80:TRP:HB2	2:B:553:HOH:O	2.18	0.43
1:B:181:MSE:HE2	1:B:198:LEU:HB2	2.01	0.43
1:A:205:THR:CB	1:A:208:ASN:HD22	2.31	0.43
1:A:139:ASN:HB3	1:A:142:SER:OG	2.19	0.43
1:B:51:GLN:OE1	1:B:104:TYR:HB3	2.19	0.43
1:B:123:VAL:O	1:B:123:VAL:HG12	2.19	0.43
1:A:170:SER:CB	1:A:208:ASN:HD21	2.16	0.42
1:B:402:LEU:O	1:B:406:VAL:HG23	2.19	0.42
1:A:383:ARG:HH11	1:A:383:ARG:HB2	1.84	0.42
1:A:355:LEU:HD12	1:A:355:LEU:HA	1.87	0.42
1:A:504:SER:O	1:A:2:GLU:HG2	2.19	0.42
1:A:130:ILE:HG12	2:A:576:HOH:O	2.19	0.42
1:A:410:MSE:O	1:A:414:ILE:HG13	2.19	0.42
1:A:431:THR:O	1:A:435:ILE:HG13	2.19	0.42
1:B:23:LYS:HE2	1:B:23:LYS:CA	2.43	0.42
1:B:353:MSE:HE2	1:B:388:MSE:HE1	2.00	0.42
1:A:109:ALA:O	1:A:113:VAL:HG23	2.20	0.42
1:A:215:ARG:HD2	1:A:255:TYR:OH	2.20	0.42
1:B:181:MSE:HE1	1:B:198:LEU:CD2	2.44	0.42
1:B:368:LEU:HD21	1:B:405:LEU:HD22	2.01	0.42
1:A:343:ASN:HB2	1:A:344:PRO:CD	2.49	0.42
1:B:427:THR:O	1:B:430:TRP:HB3	2.20	0.42
1:A:178:ILE:HA	1:A:181:MSE:HE3	2.01	0.42
1:B:206:LYS:HG3	1:B:210:ASP:OD2	2.19	0.42
1:A:47:PRO:HG3	1:A:101:THR:HB	2.01	0.42
1:B:139:ASN:HD22	1:B:140:PRO:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:HA	1:B:75:GLN:NE2	2.33	0.42
1:B:38:VAL:HA	1:B:91:VAL:HG22	2.01	0.41
1:A:394:LEU:HA	1:A:402:LEU:HD13	2.02	0.41
1:B:118:CYS:HB3	2:B:555:HOH:O	2.19	0.41
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.94	0.41
1:B:415:GLU:HG3	2:B:523:HOH:O	2.20	0.41
1:B:69:ASP:OD2	1:B:72:ILE:HD12	2.20	0.41
1:A:16:LEU:O	1:A:19:GLU:HB3	2.21	0.41
1:B:72:ILE:O	1:B:75:GLN:CG	2.68	0.41
1:B:6:ILE:CD1	1:B:24:PHE:CD2	3.03	0.41
1:B:410:MSE:O	1:B:414:ILE:HG13	2.21	0.41
1:B:188:ASN:ND2	1:B:188:ASN:N	2.55	0.41
1:A:178:ILE:HG21	1:A:217:PHE:CE2	2.55	0.41
1:A:399:PRO:O	1:A:403:LYS:HG3	2.20	0.41
1:A:118:CYS:SG	1:A:160:ASP:HB3	2.61	0.41
1:A:268:MSE:HE2	1:A:268:MSE:HB3	1.96	0.41
1:B:228:CYS:HA	1:B:229:PRO:HD3	1.82	0.41
1:B:138:THR:HG22	1:B:179:GLN:HG2	2.03	0.41
1:A:319:LEU:HD11	1:A:355:LEU:HG	2.01	0.41
1:B:206:LYS:HB2	1:B:206:LYS:HE2	1.85	0.41
1:A:74:ALA:O	1:A:78:GLN:HG2	2.20	0.41
1:A:51:GLN:CD	1:A:104:TYR:HB3	2.39	0.41
1:A:12:SER:HA	1:A:13:PRO:HD3	1.87	0.40
1:A:229:PRO:HB3	2:A:585:HOH:O	2.22	0.40
1:A:356:SER:OG	1:A:363:ILE:HD13	2.22	0.40
1:A:9:LYS:C	1:A:11:VAL:N	2.75	0.40
1:B:26:GLU:O	1:B:30:VAL:HG23	2.22	0.40
1:B:367:VAL:HG12	1:B:371:ILE:HD11	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	458/460 (100%)	436 (95%)	16 (4%)	6 (1%)	15	30
1	B	458/460 (100%)	439 (96%)	15 (3%)	4 (1%)	21	42
All	All	916/920 (100%)	875 (96%)	31 (3%)	10 (1%)	17	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ASP
1	B	447	VAL
1	A	339	ASP
1	A	361	ASP
1	A	212	GLU
1	B	212	GLU
1	B	361	ASP
1	A	335	GLU
1	B	504	SER
1	A	105	ARG

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	399/386 (103%)	389 (98%)	10 (2%)	55	81
1	B	399/386 (103%)	386 (97%)	13 (3%)	45	73
All	All	798/772 (103%)	775 (97%)	23 (3%)	50	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	46	ASN
1	A	164	GLU
1	A	184	GLU
1	A	255	TYR
1	A	298	SER

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Mol	Chain	Res	Type
1	A	305	ARG
1	A	336	ASN
1	A	417	MSE
1	A	452	ASN
1	B	3	LEU
1	B	23	LYS
1	B	32	ASN
1	B	46	ASN
1	B	84	ASP
1	B	139	ASN
1	B	164	GLU
1	B	185	GLU
1	B	188	ASN
1	B	311	SER
1	B	417	MSE
1	B	436	CYS
1	B	446	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	46	ASN
1	A	63	ASN
1	A	132	GLN
1	A	136	ASN
1	A	139	ASN
1	A	141	ASN
1	A	159	GLN
1	A	167	GLN
1	A	171	ASN
1	A	200	ASN
1	A	208	ASN
1	A	220	GLN
1	A	285	ASN
1	A	303	GLN
1	A	336	ASN
1	A	366	HIS
1	A	401	GLN
1	B	32	ASN
1	B	46	ASN
1	B	49	ASN

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Mol	Chain	Res	Type
1	B	63	ASN
1	B	75	GLN
1	B	125	GLN
1	B	139	ASN
1	B	141	ASN
1	B	167	GLN
1	B	171	ASN
1	B	179	GLN
1	B	188	ASN
1	B	208	ASN
1	B	216	HIS
1	B	220	GLN
1	B	401	GLN
1	B	452	ASN

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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.