



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:15 PM GMT

PDB ID : 1O6P
Title : IMPORTIN BETA BOUND TO A GLFG NUCLEOPORIN PEPTIDE
Authors : Bayliss, R.; Stewart, M.
Deposited on : 2002-10-10
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

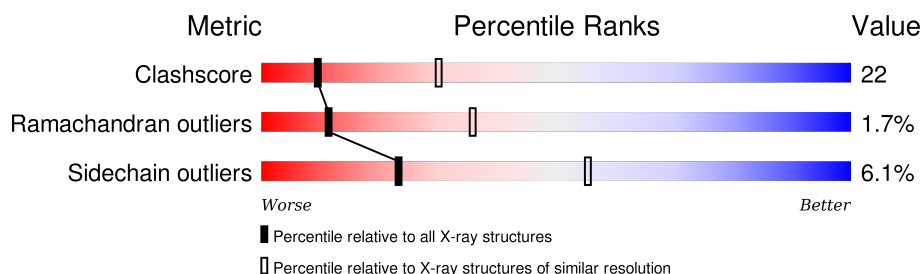
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 $\leq 5\%$. 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	442	
1	B	442	
2	C	9	
2	D	9	
2	E	9	
2	F	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7022 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-1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	1
			3441	2169	577	670	25			
1	B	441	Total	C	N	O	S	0	0	1
			3441	2169	577	670	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	HIS	GLN	CONFLICT	UNP Q14974
B	97	HIS	GLN	CONFLICT	UNP Q14974

- Molecule 2 is a protein called SYNTHETIC GLFG PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	1
			28	19	5	4			
2	D	5	Total	C	N	O	0	0	1
			28	19	5	4			
2	E	4	Total	C	N	O	0	0	1
			24	17	4	3			
2	F	4	Total	C	N	O	0	0	1
			24	17	4	3			

- Molecule 3 is water.

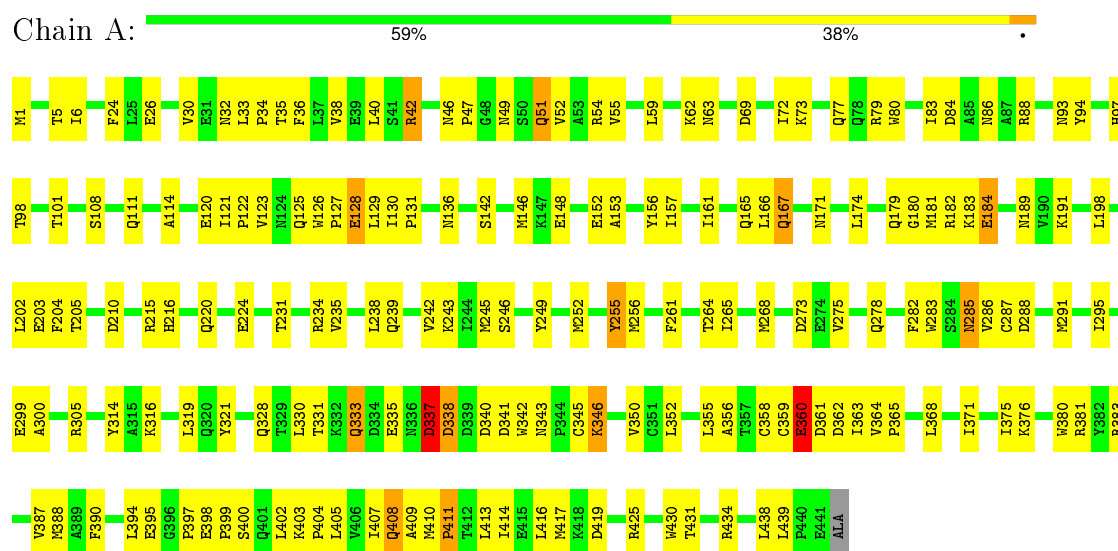
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	16	Total	O	0	0
			16	16		

3 Residue-property plots

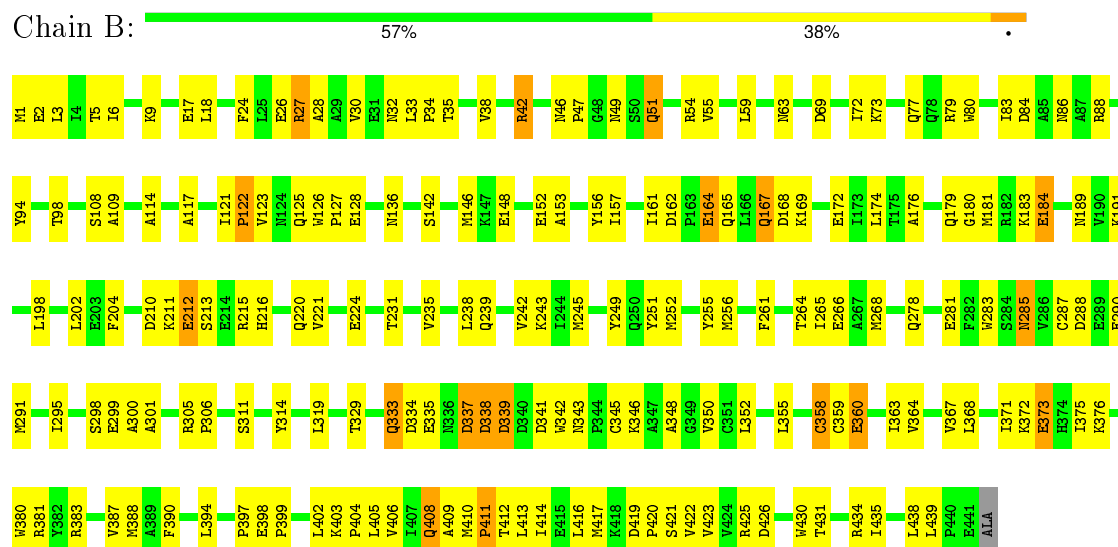
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-1 SUBUNIT

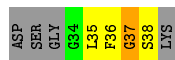


• Molecule 1: IMPORTIN BETA-1 SUBUNIT



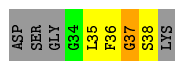
- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain C:  11% 33% 11% 44%




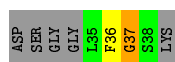
- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain D:  11% 33% 11% 44%



- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain E:  22% 11% 11% 56%



- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain F:  44% 56%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.82Å 67.03Å 129.26Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	91.8 (20.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7022	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

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	0.55	0/3505	0.69	1/4771 (0.0%)
1	B	0.56	0/3505	0.72	1/4771 (0.0%)
2	C	1.07	0/28	0.52	0/36
2	D	0.98	0/28	0.45	0/36
2	E	1.08	0/24	0.74	0/31
2	F	1.03	0/24	0.94	0/31
All	All	0.57	0/7114	0.70	2/9676 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ASP	N-CA-C	7.12	130.22	111.00
1	B	337	ASP	CB-CG-OD1	5.10	122.89	118.30

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	3441	0	3431	158	0
1	B	3441	0	3431	151	0
2	C	28	0	25	3	0
2	D	28	0	25	3	0
2	E	24	0	22	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	24	0	22	0	0
3	A	20	0	0	1	0
3	B	16	0	0	0	0
All	All	7022	0	6956	313	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 22.

All (313) 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:335:GLU:HG3	1:A:381:ARG:HH22	1.21	1.03
1:B:338:ASP:OD2	1:B:341:ASP:HB3	1.58	1.02
1:B:337:ASP:CG	1:B:338:ASP:H	1.61	0.97
1:B:338:ASP:HB2	1:B:341:ASP:HB2	1.51	0.92
1:A:338:ASP:CG	1:A:341:ASP:HB2	1.89	0.92
1:A:335:GLU:HG2	1:A:380:TRP:HZ2	1.34	0.89
1:B:338:ASP:HB2	1:B:341:ASP:CB	2.04	0.88
1:B:409:ALA:C	1:B:411:PRO:HD2	1.99	0.83
1:B:337:ASP:CG	1:B:338:ASP:N	2.33	0.82
1:A:215:ARG:HD2	1:A:255:TYR:OH	1.81	0.81
1:B:337:ASP:OD1	1:B:338:ASP:N	2.12	0.81
1:A:330:LEU:HD22	1:A:388:MET:HE3	1.63	0.80
1:B:411:PRO:HG2	1:B:412:THR:H	1.46	0.79
1:A:136:ASN:HB3	1:A:146:MET:HE2	1.64	0.79
1:B:335:GLU:HG3	1:B:381:ARG:NH2	1.99	0.77
1:B:264:THR:HG1	1:B:283:TRP:HE1	1.29	0.77
1:A:335:GLU:HG2	1:A:380:TRP:CZ2	2.18	0.76
1:A:335:GLU:HG3	1:A:381:ARG:NH2	2.00	0.75
1:B:422:VAL:HG12	1:B:426:ASP:OD2	1.87	0.75
1:B:136:ASN:HB3	1:B:146:MET:HE2	1.69	0.75
1:B:212:GLU:HB2	1:B:215:ARG:HH12	1.54	0.72
1:B:410:MET:O	1:B:414:ILE:HG12	1.91	0.71
1:A:335:GLU:CG	1:A:381:ARG:HH22	2.03	0.70
1:A:402:LEU:C	1:A:404:PRO:HD2	2.12	0.69
1:B:368:LEU:HD21	1:B:405:LEU:HD11	1.73	0.69
1:B:335:GLU:CG	1:B:381:ARG:NH2	2.56	0.69
1:A:157:ILE:O	1:A:161:ILE:HG22	1.93	0.68
1:A:404:PRO:HA	1:A:407:ILE:HG12	1.76	0.67
1:B:216:HIS:ND1	1:B:255:TYR:OH	2.26	0.67
1:B:338:ASP:CB	1:B:341:ASP:CB	2.72	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:VAL:O	1:B:123:VAL:HG12	1.95	0.67
1:B:406:VAL:HG12	1:B:410:MET:HE3	1.77	0.67
1:B:266:GLU:OE1	1:B:266:GLU:HA	1.94	0.67
1:A:368:LEU:HD21	1:A:405:LEU:HD11	1.77	0.67
1:B:383:ARG:O	1:B:387:VAL:HG23	1.94	0.67
1:B:338:ASP:CG	1:B:341:ASP:HB3	2.15	0.66
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.77	0.66
1:B:335:GLU:HG3	1:B:381:ARG:HH22	1.60	0.66
1:A:69:ASP:OD2	1:A:72:ILE:HG12	1.96	0.66
1:B:338:ASP:CB	1:B:341:ASP:HB2	2.24	0.66
1:B:167:GLN:HG3	1:B:204:PHE:HB2	1.79	0.64
1:A:47:PRO:HA	1:A:54:ARG:NH1	2.12	0.64
1:B:403:LYS:HG2	1:B:439:LEU:HD22	1.80	0.64
1:B:69:ASP:OD2	1:B:72:ILE:HG12	1.97	0.64
1:B:27:ARG:HD2	1:B:28:ALA:N	2.11	0.64
1:A:181:MET:HE1	1:A:198:LEU:HD22	1.79	0.63
1:A:410:MET:O	1:A:414:ILE:HG12	1.98	0.63
1:A:238:LEU:O	1:A:242:VAL:HG23	1.98	0.63
1:B:334:ASP:OD2	1:B:338:ASP:OD1	2.16	0.63
1:A:93:ASN:OD1	1:A:97:HIS:CD2	2.52	0.63
1:A:246:SER:HB3	1:A:285:ASN:OD1	1.99	0.62
1:B:202:LEU:HD12	1:B:243:LYS:HD3	1.81	0.61
1:B:373:GLU:O	1:B:373:GLU:HG2	2.00	0.61
1:B:388:MET:CE	1:B:430:TRP:CZ3	2.83	0.61
1:B:153:ALA:O	1:B:157:ILE:HG13	2.00	0.61
1:A:342:TRP:HH2	1:A:350:VAL:HG21	1.66	0.60
1:A:409:ALA:C	1:A:411:PRO:HD2	2.21	0.60
1:A:93:ASN:O	1:A:97:HIS:CD2	2.54	0.60
1:A:88:ARG:HH12	1:A:125:GLN:HG2	1.67	0.60
1:B:435:ILE:O	1:B:438:LEU:N	2.35	0.60
1:A:174:LEU:HD13	1:A:205:THR:HG21	1.83	0.60
1:B:338:ASP:CB	1:B:341:ASP:HB3	2.32	0.59
1:B:333:GLN:C	1:B:381:ARG:HH12	2.06	0.59
1:B:46:ASN:HB3	1:B:49:ASN:ND2	2.17	0.59
1:B:238:LEU:O	1:B:242:VAL:HG23	2.03	0.58
1:A:128:GLU:O	1:A:131:PRO:HD2	2.03	0.58
1:A:123:VAL:HG12	1:A:123:VAL:O	2.02	0.58
1:A:403:LYS:HG3	1:A:439:LEU:HD13	1.86	0.58
1:A:184:GLU:N	1:A:184:GLU:OE1	2.36	0.58
1:A:360:GLU:O	1:A:397:PRO:HG3	2.04	0.58
1:B:421:SER:O	1:B:425:ARG:N	2.24	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:CYS:O	1:A:291:MET:HG3	2.04	0.57
1:B:342:TRP:HH2	1:B:350:VAL:HG21	1.67	0.57
1:B:181:MET:HE1	1:B:198:LEU:HD22	1.86	0.57
1:B:338:ASP:HB2	1:B:341:ASP:HB3	1.85	0.57
1:A:93:ASN:ND2	1:A:97:HIS:NE2	2.53	0.57
2:C:36:PHE:O	2:C:37:GLY:C	2.43	0.57
1:A:383:ARG:O	1:A:387:VAL:HG23	2.05	0.57
1:B:388:MET:HE3	1:B:430:TRP:HZ3	1.70	0.57
1:A:265:ILE:HD13	1:A:268:MET:CE	2.34	0.57
1:A:265:ILE:HD13	1:A:268:MET:HE3	1.85	0.57
1:A:216:HIS:HD2	1:A:255:TYR:OH	1.88	0.56
1:B:404:PRO:O	1:B:408:GLN:HG2	2.05	0.56
1:A:59:LEU:CD1	1:A:62:LYS:HE3	2.34	0.56
1:A:410:MET:N	1:A:411:PRO:HD2	2.21	0.56
1:B:181:MET:HE2	1:B:198:LEU:HB2	1.86	0.56
2:D:36:PHE:O	2:D:37:GLY:C	2.44	0.56
1:A:404:PRO:O	1:A:407:ILE:HB	2.05	0.56
1:A:343:ASN:ND2	1:A:345:CYS:HB3	2.20	0.56
1:B:265:ILE:HD13	1:B:268:MET:CE	2.36	0.56
1:A:234:ARG:NH1	3:A:2017:HOH:O	2.39	0.56
1:B:183:LYS:HD2	1:B:224:GLU:HB3	1.86	0.56
1:A:153:ALA:O	1:A:157:ILE:HG13	2.07	0.55
1:A:46:ASN:HB3	1:A:49:ASN:ND2	2.21	0.55
1:B:419:ASP:CG	1:B:420:PRO:HD2	2.27	0.55
1:A:387:VAL:CG2	1:A:416:LEU:HD13	2.36	0.55
1:A:181:MET:HE2	1:A:198:LEU:HB2	1.88	0.55
1:A:93:ASN:CG	1:A:97:HIS:NE2	2.60	0.55
1:B:42:ARG:HD3	1:B:94:TYR:CZ	2.43	0.54
1:B:169:LYS:HA	1:B:172:GLU:OE1	2.08	0.54
1:B:419:ASP:OD1	1:B:420:PRO:HD2	2.07	0.54
1:B:388:MET:HE1	1:B:430:TRP:CZ3	2.41	0.54
1:A:335:GLU:OE2	1:A:381:ARG:NH1	2.40	0.54
1:B:18:LEU:C	1:B:18:LEU:HD23	2.27	0.54
1:A:338:ASP:OD2	1:A:341:ASP:HB2	2.08	0.54
2:C:36:PHE:O	2:C:38:SER:N	2.41	0.54
1:B:295:ILE:HG22	1:B:299:GLU:OE2	2.08	0.53
1:B:88:ARG:HH12	1:B:125:GLN:HG2	1.72	0.53
1:B:220:GLN:O	1:B:224:GLU:HG3	2.08	0.53
1:A:126:TRP:HD1	1:A:128:GLU:HG3	1.73	0.53
1:B:265:ILE:HA	1:B:268:MET:HE3	1.89	0.53
1:A:338:ASP:C	1:A:340:ASP:H	2.10	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:HG22	1:A:299:GLU:OE2	2.08	0.53
1:A:26:GLU:O	1:A:30:VAL:HG23	2.09	0.53
1:B:430:TRP:CZ2	1:B:434:ARG:HD2	2.45	0.52
1:B:380:TRP:HZ3	1:B:423:VAL:HG11	1.74	0.52
1:B:98:THR:HG21	1:B:109:ALA:HB2	1.91	0.52
1:A:202:LEU:HD12	1:A:243:LYS:HD3	1.91	0.52
1:B:430:TRP:CE2	1:B:434:ARG:HD2	2.44	0.52
1:A:51:GLN:HG3	1:A:52:VAL:N	2.25	0.52
1:A:1:MET:HA	1:A:5:THR:HG21	1.92	0.52
2:D:36:PHE:O	2:D:38:SER:N	2.43	0.52
1:B:184:GLU:OE1	1:B:184:GLU:N	2.43	0.52
1:B:410:MET:N	1:B:411:PRO:HD2	2.23	0.52
1:A:93:ASN:OD1	1:A:97:HIS:NE2	2.43	0.52
1:B:122:PRO:HA	1:B:165:GLN:NE2	2.24	0.52
1:B:388:MET:HE3	1:B:430:TRP:CZ3	2.43	0.52
1:B:80:TRP:O	1:B:88:ARG:HD3	2.10	0.52
1:A:203:GLU:OE2	1:A:243:LYS:HE2	2.10	0.52
1:A:265:ILE:HA	1:A:268:MET:CE	2.40	0.52
1:B:290:GLU:HG2	1:B:311:SER:OG	2.10	0.52
1:A:183:LYS:HD2	1:A:224:GLU:HB3	1.92	0.51
1:B:84:ASP:OD2	1:B:86:ASN:HB2	2.11	0.51
1:A:343:ASN:HD21	1:A:345:CYS:HB3	1.75	0.51
1:B:235:VAL:O	1:B:239:GLN:HG3	2.10	0.51
1:A:403:LYS:O	1:A:407:ILE:HG12	2.09	0.51
1:B:265:ILE:HA	1:B:268:MET:CE	2.41	0.51
1:A:73:LYS:O	1:A:77:GLN:HG3	2.10	0.51
1:A:59:LEU:HD12	1:A:62:LYS:HE3	1.93	0.51
1:B:343:ASN:ND2	1:B:345:CYS:HB3	2.26	0.51
1:B:335:GLU:HG2	1:B:380:TRP:HZ2	1.76	0.51
1:A:245:MET:HE3	1:A:252:MET:HG3	1.93	0.51
1:A:36:PHE:CZ	1:A:40:LEU:HD11	2.46	0.51
1:B:179:GLN:HA	1:B:179:GLN:NE2	2.26	0.51
1:B:406:VAL:HG12	1:B:410:MET:CE	2.40	0.51
1:A:121:ILE:N	1:A:122:PRO:HD2	2.26	0.51
1:B:264:THR:OG1	1:B:283:TRP:NE1	2.30	0.50
1:B:157:ILE:O	1:B:161:ILE:HG22	2.11	0.50
1:A:430:TRP:CE2	1:A:434:ARG:HD2	2.46	0.50
1:A:235:VAL:O	1:A:239:GLN:HG3	2.10	0.50
1:A:256:MET:HE1	1:A:283:TRP:CZ2	2.46	0.50
1:B:411:PRO:HG2	1:B:412:THR:N	2.23	0.50
1:A:182:ARG:NE	1:A:184:GLU:OE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLN:HE22	1:A:388:MET:CE	2.24	0.50
1:A:403:LYS:N	1:A:404:PRO:HD2	2.25	0.50
1:A:59:LEU:HG	1:A:63:ASN:HD21	1.77	0.50
1:B:51:GLN:O	1:B:55:VAL:HG23	2.11	0.50
1:A:42:ARG:HD3	1:A:94:TYR:CZ	2.46	0.50
1:B:117:ALA:HB1	1:B:121:ILE:HD12	1.94	0.50
1:A:265:ILE:HA	1:A:268:MET:HE2	1.94	0.50
1:A:59:LEU:O	1:A:63:ASN:ND2	2.44	0.50
1:A:398:GLU:HG2	1:A:400:SER:OG	2.12	0.50
1:A:256:MET:HG2	1:A:314:TYR:CD1	2.48	0.49
1:A:80:TRP:O	1:A:88:ARG:HD3	2.12	0.49
1:A:33:LEU:HB3	1:A:34:PRO:HD3	1.93	0.49
1:B:47:PRO:HA	1:B:54:ARG:NH1	2.26	0.49
1:A:430:TRP:CZ2	1:A:434:ARG:HD2	2.47	0.49
1:A:239:GLN:HG2	1:A:278:GLN:NE2	2.28	0.49
1:A:179:GLN:HA	1:A:179:GLN:NE2	2.26	0.49
1:A:316:LYS:HA	1:A:359:CYS:SG	2.53	0.49
1:A:399:PRO:HA	1:A:439:LEU:HD21	1.95	0.49
1:A:390:PHE:O	1:A:394:LEU:HG	2.13	0.49
1:B:73:LYS:O	1:B:77:GLN:HG3	2.13	0.48
1:B:417:MET:O	1:B:425:ARG:HG2	2.13	0.48
1:A:404:PRO:HA	1:A:407:ILE:CG1	2.43	0.48
1:B:26:GLU:O	1:B:30:VAL:HG23	2.13	0.48
1:A:148:GLU:OE2	1:A:189:ASN:HB3	2.13	0.48
1:B:383:ARG:NH1	1:B:419:ASP:OD1	2.46	0.48
1:B:287:CYS:O	1:B:291:MET:HG3	2.13	0.48
1:A:33:LEU:HD23	1:A:83:ILE:HD11	1.95	0.48
1:B:339:ASP:C	1:B:339:ASP:OD1	2.52	0.48
1:B:148:GLU:OE2	1:B:189:ASN:HB3	2.13	0.48
1:A:337:ASP:HB3	1:A:338:ASP:OD1	2.13	0.48
1:B:122:PRO:CB	1:B:165:GLN:HE22	2.27	0.48
1:A:300:ALA:HB1	1:A:305:ARG:O	2.14	0.48
1:A:404:PRO:CA	1:A:407:ILE:HG12	2.44	0.48
1:B:121:ILE:N	1:B:122:PRO:HD2	2.29	0.48
1:A:338:ASP:OD1	1:A:341:ASP:HB2	2.12	0.48
1:A:387:VAL:HG21	1:A:416:LEU:HD13	1.96	0.47
1:A:408:GLN:H	1:A:408:GLN:HG2	1.42	0.47
1:B:245:MET:HE2	1:B:249:TYR:CD2	2.50	0.47
1:A:364:VAL:HB	1:A:365:PRO:CD	2.45	0.47
1:A:126:TRP:CD1	1:A:128:GLU:HG3	2.49	0.47
1:B:114:ALA:CB	1:B:156:TYR:HB3	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:NH1	1:A:419:ASP:OD1	2.48	0.47
1:B:413:LEU:HD11	1:B:431:THR:HG21	1.95	0.47
1:B:211:LYS:HE2	1:B:213:SER:HB3	1.96	0.47
1:B:403:LYS:N	1:B:404:PRO:HD2	2.29	0.46
1:A:383:ARG:HH11	1:A:419:ASP:CG	2.18	0.46
1:A:231:THR:O	1:A:235:VAL:HG23	2.15	0.46
1:A:220:GLN:O	1:A:224:GLU:HG3	2.16	0.46
1:B:1:MET:HA	1:B:5:THR:HG21	1.98	0.46
1:B:33:LEU:HD22	1:B:79:ARG:HD2	1.97	0.46
1:A:171:ASN:ND2	2:E:37:GLY:HA2	2.31	0.46
1:B:402:LEU:O	1:B:406:VAL:HG23	2.16	0.46
1:A:410:MET:CE	1:A:414:ILE:HD11	2.46	0.46
1:B:363:ILE:HG23	1:B:364:VAL:N	2.31	0.46
1:A:414:ILE:HA	1:A:417:MET:HE2	1.98	0.46
1:A:371:ILE:HD13	1:A:390:PHE:HB2	1.96	0.46
1:B:343:ASN:HD21	1:B:345:CYS:HB3	1.79	0.46
1:B:300:ALA:HB1	1:B:305:ARG:O	2.16	0.46
1:B:390:PHE:O	1:B:394:LEU:HG	2.16	0.46
1:A:333:GLN:O	1:A:381:ARG:NH2	2.45	0.45
1:B:422:VAL:HA	1:B:425:ARG:HB2	1.98	0.45
1:B:265:ILE:HD13	1:B:268:MET:HE3	1.97	0.45
1:A:84:ASP:OD2	1:A:86:ASN:HB2	2.16	0.45
1:B:6:ILE:HG21	1:B:24:PHE:CD2	2.51	0.45
1:B:387:VAL:CG2	1:B:416:LEU:HD13	2.46	0.45
1:A:362:ASP:OD1	1:A:362:ASP:N	2.49	0.45
1:A:395:GLU:HB2	1:A:434:ARG:HH22	1.82	0.45
1:B:422:VAL:O	1:B:426:ASP:N	2.35	0.45
1:A:34:PRO:O	1:A:38:VAL:HG23	2.16	0.45
1:A:171:ASN:HD22	2:E:36:PHE:C	2.20	0.45
1:B:285:ASN:HA	1:B:285:ASN:HD22	1.54	0.44
1:B:117:ALA:HB1	1:B:121:ILE:CD1	2.47	0.44
1:B:329:THR:HG21	1:B:348:ALA:HB2	1.98	0.44
1:A:179:GLN:HE21	1:A:179:GLN:HA	1.82	0.44
1:B:383:ARG:HH11	1:B:419:ASP:CG	2.21	0.44
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.87	0.44
1:A:114:ALA:CB	1:A:156:TYR:HB3	2.48	0.44
1:A:333:GLN:NE2	1:A:388:MET:HE1	2.33	0.44
1:A:181:MET:CE	1:A:198:LEU:HD22	2.46	0.44
1:A:261:PHE:HZ	1:A:321:TYR:CD1	2.36	0.44
1:B:79:ARG:O	1:B:83:ILE:HG13	2.18	0.44
1:A:167:GLN:HG3	1:A:204:PHE:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:PRO:CG	1:B:412:THR:H	2.22	0.43
1:A:136:ASN:CB	1:A:146:MET:HE2	2.42	0.43
1:B:245:MET:HE3	1:B:252:MET:HG3	2.00	0.43
1:B:35:THR:HG23	2:C:35:LEU:HD21	2.00	0.43
1:A:282:PHE:O	1:A:286:VAL:HG23	2.18	0.43
1:A:234:ARG:NH2	1:A:275:VAL:HG11	2.33	0.43
1:A:338:ASP:C	1:A:340:ASP:N	2.72	0.43
1:A:413:LEU:HD11	1:A:431:THR:HG21	2.01	0.43
1:B:333:GLN:CB	1:B:381:ARG:NH1	2.81	0.43
1:A:410:MET:HE3	1:A:414:ILE:HD11	1.99	0.43
1:A:33:LEU:HD22	1:A:79:ARG:HD2	2.01	0.43
1:B:319:LEU:HD13	1:B:359:CYS:SG	2.59	0.43
1:B:412:THR:O	1:B:416:LEU:HG	2.18	0.43
1:B:176:ALA:O	1:B:179:GLN:HB3	2.18	0.43
1:B:179:GLN:HA	1:B:179:GLN:HE21	1.82	0.43
1:B:256:MET:HG2	1:B:314:TYR:CD1	2.53	0.43
1:B:215:ARG:NH2	1:B:251:TYR:CD1	2.87	0.43
1:A:342:TRP:CZ3	1:A:346:LYS:HB3	2.54	0.43
1:B:181:MET:HB3	1:B:221:VAL:CG1	2.49	0.43
1:A:375:ILE:HG23	1:A:376:LYS:HG3	2.01	0.43
1:A:380:TRP:CZ2	1:A:381:ARG:NH1	2.87	0.42
1:B:245:MET:HE3	1:B:249:TYR:HA	2.01	0.42
1:B:261:PHE:O	1:B:265:ILE:HG12	2.18	0.42
1:B:373:GLU:O	1:B:373:GLU:CG	2.67	0.42
1:A:387:VAL:HG22	1:A:416:LEU:HD13	2.00	0.42
1:B:126:TRP:N	1:B:127:PRO:CD	2.81	0.42
1:A:328:GLN:O	1:A:331:THR:HB	2.20	0.42
1:A:261:PHE:O	1:A:265:ILE:HG12	2.20	0.42
1:B:180:GLY:O	1:B:191:LYS:HA	2.19	0.42
1:B:168:ASP:N	1:B:168:ASP:OD1	2.42	0.42
1:A:245:MET:HE2	1:A:249:TYR:CD2	2.55	0.42
1:A:42:ARG:HG2	1:A:94:TYR:CE2	2.54	0.42
1:B:305:ARG:HB2	1:B:306:PRO:HD2	2.00	0.42
1:B:333:GLN:O	1:B:381:ARG:NH1	2.39	0.42
1:B:121:ILE:C	1:B:123:VAL:H	2.22	0.42
1:A:419:ASP:O	1:A:425:ARG:CD	2.67	0.42
1:A:245:MET:CE	1:A:252:MET:HG3	2.50	0.42
1:B:414:ILE:HA	1:B:417:MET:HE2	2.02	0.42
1:A:88:ARG:HH12	1:A:125:GLN:CG	2.32	0.42
1:B:46:ASN:HB3	1:B:49:ASN:HD21	1.83	0.42
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HG21	1:A:24:PHE:CD2	2.55	0.42
1:A:165:GLN:O	1:A:166:LEU:HG	2.19	0.42
1:B:59:LEU:HG	1:B:63:ASN:HD21	1.85	0.42
1:A:356:ALA:O	1:A:360:GLU:HA	2.19	0.41
1:B:9:LYS:HD3	1:B:17:GLU:CG	2.49	0.41
1:B:152:GLU:O	1:B:156:TYR:CD2	2.73	0.41
1:B:298:SER:O	1:B:301:ALA:HB3	2.19	0.41
1:B:162:ASP:C	1:B:164:GLU:N	2.72	0.41
1:B:122:PRO:HB3	1:B:165:GLN:HE22	1.85	0.41
1:B:98:THR:CG2	1:B:109:ALA:HB2	2.49	0.41
1:A:79:ARG:O	1:A:83:ILE:HG13	2.20	0.41
1:B:33:LEU:HD23	1:B:83:ILE:HD11	2.02	0.41
1:A:35:THR:HG23	2:D:35:LEU:HD21	2.01	0.41
1:A:416:LEU:HA	1:A:419:ASP:HB2	2.03	0.41
1:B:34:PRO:O	1:B:38:VAL:HG23	2.21	0.41
1:B:367:VAL:HG12	1:B:371:ILE:HD11	2.02	0.41
1:A:179:GLN:CA	1:A:179:GLN:NE2	2.84	0.41
1:A:363:ILE:HG23	1:A:364:VAL:N	2.35	0.41
1:A:98:THR:O	1:A:101:THR:HG23	2.21	0.41
1:A:264:THR:HG21	1:A:282:PHE:CD2	2.55	0.41
1:A:346:LYS:O	1:A:350:VAL:HG23	2.21	0.41
1:A:121:ILE:C	1:A:123:VAL:H	2.24	0.41
1:B:360:GLU:O	1:B:397:PRO:HG3	2.19	0.41
1:B:231:THR:O	1:B:235:VAL:HG23	2.21	0.41
1:B:375:ILE:HG23	1:B:376:LYS:HG3	2.03	0.41
1:A:180:GLY:O	1:A:191:LYS:HA	2.21	0.41
1:B:398:GLU:HA	1:B:399:PRO:HD3	1.94	0.41
1:A:403:LYS:HE2	1:A:439:LEU:HB3	2.03	0.40
1:A:120:GLU:HB3	1:A:125:GLN:HB3	2.03	0.40
1:A:51:GLN:O	1:A:55:VAL:HG23	2.22	0.40
1:A:264:THR:HG21	1:A:282:PHE:CE2	2.56	0.40
1:A:361:ASP:C	1:A:363:ILE:H	2.25	0.40
1:B:338:ASP:O	1:B:338:ASP:OD1	2.39	0.40
1:A:398:GLU:HG3	1:A:399:PRO:HD2	2.02	0.40
1:A:398:GLU:HA	1:A:399:PRO:HD3	1.89	0.40
1:B:358:CYS:C	1:B:360:GLU:H	2.24	0.40
1:A:148:GLU:O	1:A:152:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	439/442 (99%)	398 (91%)	35 (8%)	6 (1%)	14	42
1	B	439/442 (99%)	400 (91%)	33 (8%)	6 (1%)	14	42
2	C	3/9 (33%)	2 (67%)	0	1 (33%)	0	0
2	D	3/9 (33%)	2 (67%)	0	1 (33%)	0	0
2	E	2/9 (22%)	1 (50%)	0	1 (50%)	0	0
2	F	2/9 (22%)	2 (100%)	0	0	100	100
All	All	888/920 (96%)	805 (91%)	68 (8%)	15 (2%)	11	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLU
1	A	438	LEU
1	B	360	GLU
2	C	37	GLY
2	D	37	GLY
1	A	129	LEU
1	A	338	ASP
1	B	338	ASP
1	B	373	GLU
1	B	411	PRO
2	E	37	GLY
1	B	372	LYS
1	A	319	LEU
1	A	411	PRO
1	B	122	PRO

5.3.2 Protein sidechains ⓘ

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	381/382 (100%)	359 (94%)	22 (6%)	25	57
1	B	381/382 (100%)	356 (93%)	25 (7%)	21	51
2	C	2/6 (33%)	2 (100%)	0	100	100
2	D	2/6 (33%)	2 (100%)	0	100	100
2	E	2/6 (33%)	2 (100%)	0	100	100
2	F	2/6 (33%)	2 (100%)	0	100	100
All	All	770/788 (98%)	723 (94%)	47 (6%)	23	55

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	42	ARG
1	A	51	GLN
1	A	108	SER
1	A	111	GLN
1	A	127	PRO
1	A	128	GLU
1	A	142	SER
1	A	167	GLN
1	A	184	GLU
1	A	210	ASP
1	A	255	TYR
1	A	273	ASP
1	A	285	ASN
1	A	288	ASP
1	A	333	GLN
1	A	337	ASP
1	A	346	LYS
1	A	352	LEU
1	A	358	CYS
1	A	360	GLU
1	A	408	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2	GLU
1	B	3	LEU
1	B	27	ARG
1	B	32	ASN
1	B	42	ARG
1	B	51	GLN
1	B	108	SER
1	B	128	GLU
1	B	142	SER
1	B	164	GLU
1	B	167	GLN
1	B	174	LEU
1	B	184	GLU
1	B	210	ASP
1	B	212	GLU
1	B	278	GLN
1	B	281	GLU
1	B	285	ASN
1	B	288	ASP
1	B	333	GLN
1	B	339	ASP
1	B	346	LYS
1	B	352	LEU
1	B	358	CYS
1	B	408	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	49	ASN
1	A	63	ASN
1	A	111	GLN
1	A	141	ASN
1	A	171	ASN
1	A	179	GLN
1	A	208	ASN
1	A	216	HIS
1	A	240	ASN
1	A	278	GLN
1	A	333	GLN
1	A	401	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	ASN
1	B	49	ASN
1	B	63	ASN
1	B	97	HIS
1	B	141	ASN
1	B	165	GLN
1	B	171	ASN
1	B	208	ASN
1	B	285	ASN
1	B	328	GLN
1	B	374	HIS
1	B	377	ASN
1	B	401	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](#)

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.