



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 05:54 AM EDT

PDB ID : 1P9M
Title : Crystal structure of the hexameric human IL-6/IL-6 alpha receptor/gp130 complex
Authors : Boulanger, M.J.; Chow, D.C.; Brevnova, E.E.; Garcia, K.C.
Deposited on : 2003-05-12
Resolution : 3.65 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

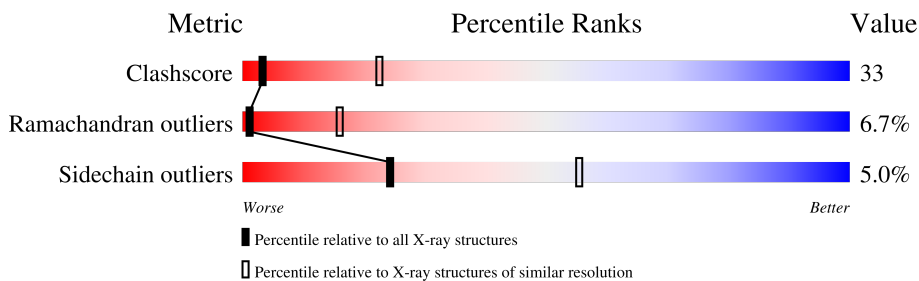
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	299	 47% 46% 6%
2	B	186	 46% 38% 12%
3	C	201	 48% 45% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5322 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 Interleukin-6 receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2390	1525	393	460	12	91	0	0

- Molecule 2 is a protein called Interleukin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	163	1309	820	225	256	8	109	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ALA	-	cloning artifact	UNP P05231
B	0	PRO	-	cloning artifact	UNP P05231

- Molecule 3 is a protein called Interleukin-6 receptor alpha chain.

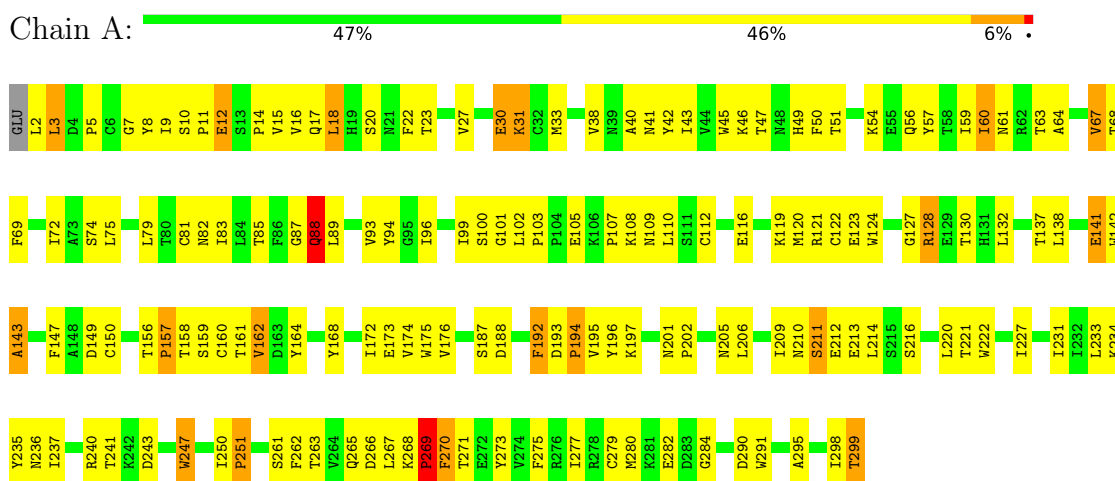
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	201	1623	1027	284	302	10	27	0	0

3 Residue-property plots [i](#)

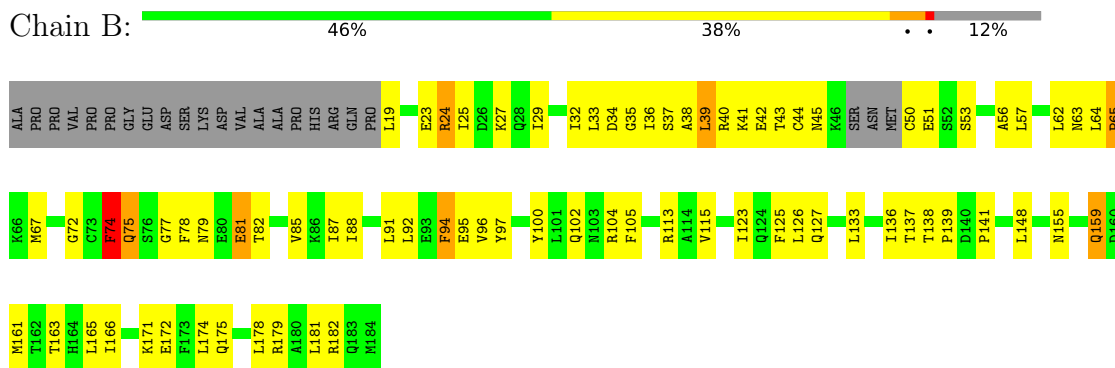
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

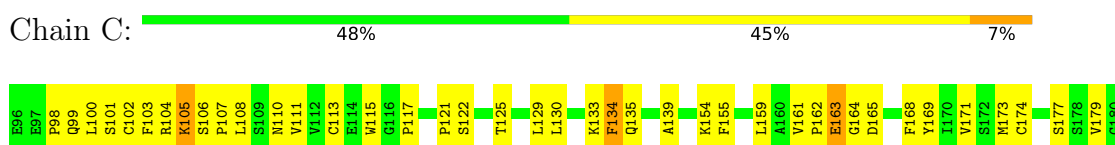
- Molecule 1: Interleukin-6 receptor beta chain

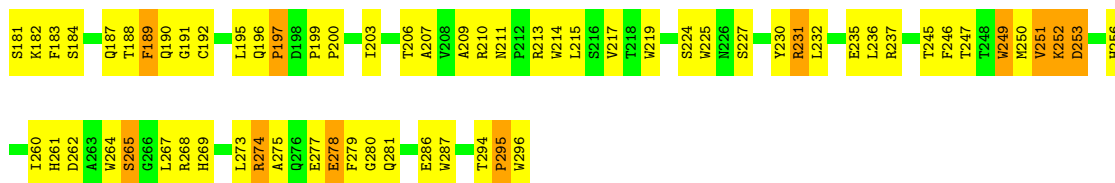


- Molecule 2: Interleukin-6



- Molecule 3: Interleukin-6 receptor alpha chain





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	279.80Å 279.80Å 96.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.65	Depositor
% Data completeness (in resolution range)	98.2 (19.99-3.65)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.282 , 0.334	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å ²)	117.0	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	0.27	0/2452	0.51	0/3340
2	B	0.37	1/1323 (0.1%)	0.53	0/1775
3	C	0.35	0/1674	0.61	3/2277 (0.1%)
All	All	0.32	1/5449 (0.0%)	0.55	3/7392 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	95	GLU	CD-OE2	6.87	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	249	TRP	CB-CA-C	-7.74	94.92	110.40
3	C	249	TRP	CG-CD2-CE3	6.01	139.31	133.90
3	C	249	TRP	CA-C-N	5.26	128.78	117.20

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	2390	0	2334	142	0
2	B	1309	0	1327	86	0
3	C	1623	0	1541	115	0
All	All	5322	0	5202	329	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 33.

All (329) 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)
2:B:137:THR:O	2:B:139:PRO:HD3	1.51	1.07
1:A:211:SER:HB3	3:C:245:THR:HG21	1.40	1.03
3:C:100:LEU:HD11	3:C:113:CYS:HB3	1.41	1.02
3:C:236:LEU:HD23	3:C:237:ARG:N	1.80	0.96
1:A:209:ILE:HG22	1:A:211:SER:OG	1.70	0.91
2:B:104:ARG:HD2	2:B:163:THR:HG21	1.53	0.91
3:C:278:GLU:HG3	3:C:279:PHE:HD1	1.37	0.89
2:B:178:LEU:HD23	3:C:279:PHE:HZ	1.37	0.87
3:C:278:GLU:HG3	3:C:279:PHE:CD1	2.09	0.86
2:B:171:LYS:HG2	2:B:175:GLN:HE21	1.41	0.83
1:A:138:LEU:HB3	1:A:150:CYS:HB3	1.62	0.82
3:C:133:LYS:HG3	3:C:169:TYR:HE2	1.42	0.82
2:B:137:THR:O	2:B:139:PRO:CD	2.31	0.78
2:B:104:ARG:HH21	2:B:159:GLN:HE22	1.32	0.77
1:A:209:ILE:CG2	1:A:211:SER:OG	2.34	0.76
1:A:107:PRO:HB2	1:A:187:SER:HB2	1.68	0.74
1:A:202:PRO:HB3	1:A:290:ASP:O	1.87	0.74
1:A:101:GLY:HA3	1:A:132:LEU:HD11	1.68	0.74
2:B:74:PHE:HD2	3:C:163:GLU:HB3	1.51	0.74
1:A:116:GLU:HB3	1:A:201:ASN:OD1	1.87	0.74
3:C:98:PRO:HB2	3:C:184:SER:N	2.03	0.73
3:C:264:TRP:HB3	3:C:267:LEU:HD12	1.69	0.73
2:B:104:ARG:CD	2:B:163:THR:HG21	2.19	0.72
2:B:182:ARG:NH1	3:C:231:ARG:HG2	2.03	0.72
3:C:213:ARG:NH1	3:C:265:SER:H	1.87	0.72
2:B:74:PHE:HE2	3:C:164:GLY:HA3	1.55	0.71
1:A:216:SER:HA	1:A:267:LEU:HB2	1.73	0.70
2:B:104:ARG:HD2	2:B:163:THR:CG2	2.22	0.70
3:C:268:ARG:HA	3:C:294:THR:HG22	1.74	0.70
1:A:237:ILE:HB	1:A:250:ILE:HD12	1.74	0.70
2:B:50:CYS:N	2:B:53:SER:HG	1.88	0.70
3:C:134:PHE:HD1	3:C:168:PHE:HB2	1.57	0.69
1:A:27:VAL:HG12	1:A:64:ALA:HB2	1.74	0.69
3:C:219:TRP:HH2	3:C:251:VAL:HG21	1.58	0.69
3:C:206:THR:HG22	3:C:207:ALA:H	1.56	0.69
1:A:119:LYS:H	1:A:119:LYS:HD2	1.58	0.68
3:C:192:CYS:HB2	3:C:281:GLN:OE1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ARG:NH2	2:B:159:GLN:HE22	1.90	0.67
2:B:104:ARG:HH21	2:B:159:GLN:NE2	1.92	0.66
3:C:267:LEU:H	3:C:295:PRO:HD2	1.59	0.66
3:C:252:LYS:HG3	3:C:253:ASP:H	1.59	0.66
3:C:219:TRP:CH2	3:C:251:VAL:HG21	2.31	0.65
2:B:97:TYR:HB3	2:B:166:ILE:HD13	1.79	0.65
2:B:96:VAL:HG13	2:B:97:TYR:H	1.61	0.65
2:B:126:LEU:HD21	2:B:181:LEU:HD11	1.79	0.64
3:C:277:GLU:OE1	3:C:281:GLN:HB3	1.97	0.64
2:B:40:ARG:O	2:B:43:THR:HG22	1.98	0.64
3:C:195:LEU:HD12	3:C:196:GLN:H	1.62	0.64
3:C:102:CYS:HA	3:C:113:CYS:HA	1.78	0.64
3:C:125:THR:HA	3:C:177:SER:HB3	1.79	0.64
1:A:193:ASP:OD1	1:A:195:VAL:HG12	1.97	0.63
1:A:209:ILE:HG22	1:A:211:SER:H	1.63	0.63
3:C:104:ARG:HG2	3:C:106:SER:O	1.98	0.63
2:B:23:GLU:C	2:B:25:ILE:H	2.02	0.63
2:B:67:MET:HB3	2:B:74:PHE:CE1	2.34	0.62
1:A:250:ILE:HG23	1:A:251:PRO:HD2	1.79	0.62
1:A:234:LYS:HB2	1:A:282:GLU:HA	1.79	0.62
1:A:206:LEU:HD23	1:A:206:LEU:H	1.64	0.62
3:C:232:LEU:HG	3:C:275:ALA:HB1	1.82	0.62
1:A:250:ILE:HD13	1:A:262:PHE:HE2	1.63	0.62
1:A:211:SER:CB	3:C:245:THR:HG21	2.25	0.61
2:B:67:MET:HB3	2:B:74:PHE:HE1	1.63	0.61
3:C:105:LYS:HB3	3:C:224:SER:HB2	1.81	0.61
2:B:182:ARG:HH12	3:C:231:ARG:HG2	1.63	0.61
1:A:222:TRP:NE1	1:A:235:TYR:CE2	2.67	0.61
3:C:162:PRO:HG2	3:C:165:ASP:HB2	1.83	0.60
3:C:203:ILE:HD12	3:C:273:LEU:HD23	1.82	0.60
2:B:136:ILE:HG22	2:B:138:THR:H	1.66	0.60
3:C:206:THR:HG22	3:C:207:ALA:N	2.14	0.60
1:A:147:PHE:HB3	1:A:164:TYR:CE2	2.36	0.60
2:B:139:PRO:O	2:B:141:PRO:HD3	2.01	0.60
1:A:141:GLU:O	1:A:172:ILE:HD12	2.01	0.60
1:A:172:ILE:HG22	1:A:194:PRO:HD3	1.84	0.60
1:A:241:THR:HG22	1:A:243:ASP:H	1.66	0.60
1:A:38:VAL:HA	1:A:42:TYR:HD2	1.67	0.59
1:A:195:VAL:HG13	1:A:196:TYR:CD2	2.38	0.59
2:B:36:ILE:H	2:B:36:ILE:HD12	1.67	0.59
1:A:75:LEU:H	1:A:75:LEU:HD23	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:N	1:A:132:LEU:HD12	2.18	0.58
3:C:197:PRO:HG3	3:C:225:TRP:CZ3	2.39	0.58
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.69	0.58
1:A:172:ILE:CG2	1:A:194:PRO:HD3	2.34	0.58
1:A:38:VAL:HA	1:A:42:TYR:CD2	2.38	0.57
2:B:81:GLU:HG3	2:B:133:LEU:HD22	1.87	0.57
3:C:209:ALA:HA	3:C:296:TRP:CD1	2.40	0.57
3:C:237:ARG:HA	3:C:247:THR:O	2.05	0.57
3:C:199:PRO:HG3	3:C:286:GLU:O	2.04	0.57
1:A:121:ARG:HD3	1:A:161:THR:OG1	2.05	0.57
1:A:101:GLY:HA3	1:A:132:LEU:CD1	2.35	0.57
2:B:161:MET:O	2:B:165:LEU:HG	2.04	0.57
1:A:75:LEU:HD23	1:A:75:LEU:N	2.19	0.57
2:B:79:ASN:HB3	2:B:82:THR:OG1	2.05	0.57
1:A:240:ARG:HG2	1:A:247:TRP:CZ3	2.39	0.56
1:A:269:PRO:O	1:A:299:THR:HG23	2.05	0.56
1:A:45:TRP:CE2	1:A:67:VAL:HG22	2.40	0.56
3:C:133:LYS:HG3	3:C:169:TYR:CE2	2.32	0.56
3:C:100:LEU:H	3:C:184:SER:HB2	1.71	0.56
3:C:173:MET:HG2	3:C:174:CYS:H	1.71	0.55
2:B:75:GLN:CA	2:B:75:GLN:HE21	2.17	0.55
2:B:171:LYS:HE3	2:B:175:GLN:NE2	2.21	0.55
1:A:59:ILE:N	1:A:59:ILE:HD12	2.22	0.55
1:A:12:GLU:O	1:A:14:PRO:HD3	2.06	0.55
1:A:54:LYS:HA	1:A:57:TYR:CD1	2.42	0.55
3:C:98:PRO:O	3:C:184:SER:HA	2.07	0.55
2:B:102:GLN:HE22	2:B:113:ARG:HA	1.71	0.55
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.08	0.54
2:B:96:VAL:HG13	2:B:97:TYR:N	2.22	0.54
3:C:213:ARG:HH11	3:C:265:SER:H	1.54	0.54
3:C:236:LEU:HD23	3:C:237:ARG:H	1.69	0.54
1:A:88:GLN:OE1	1:A:88:GLN:O	2.25	0.54
1:A:101:GLY:CA	1:A:132:LEU:HD11	2.36	0.54
1:A:102:LEU:O	1:A:130:THR:HG23	2.07	0.54
1:A:263:THR:HB	3:C:262:ASP:HB2	1.89	0.54
2:B:171:LYS:CG	2:B:175:GLN:HE21	2.19	0.54
1:A:5:PRO:C	1:A:7:GLY:H	2.11	0.54
2:B:74:PHE:CE2	3:C:164:GLY:HA3	2.41	0.54
1:A:69:PHE:HZ	1:A:79:LEU:HD21	1.72	0.54
3:C:203:ILE:HD13	3:C:219:TRP:HB3	1.88	0.54
2:B:65:PRO:HB2	2:B:94:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ASP:O	2:B:37:SER:HB2	2.08	0.53
3:C:235:GLU:HG3	3:C:250:MET:HG3	1.89	0.53
1:A:15:VAL:HG22	1:A:99:ILE:HG13	1.89	0.53
2:B:104:ARG:HH11	2:B:104:ARG:HB3	1.72	0.53
3:C:171:VAL:HG23	3:C:187:GLN:HB3	1.90	0.53
1:A:172:ILE:HG23	1:A:192:PHE:CE2	2.43	0.53
2:B:74:PHE:H	2:B:74:PHE:HD1	1.56	0.53
3:C:215:LEU:HB2	3:C:260:ILE:HD12	1.91	0.53
3:C:277:GLU:O	3:C:280:GLY:N	2.42	0.53
1:A:157:PRO:HG2	1:A:158:THR:H	1.73	0.52
1:A:119:LYS:HD2	1:A:119:LYS:N	2.24	0.52
1:A:250:ILE:HD13	1:A:262:PHE:CE2	2.45	0.52
1:A:268:LYS:O	1:A:269:PRO:O	2.27	0.52
3:C:273:LEU:O	3:C:274:ARG:HB3	2.10	0.52
2:B:39:LEU:HD11	2:B:115:VAL:HG21	1.92	0.52
3:C:232:LEU:HD12	3:C:277:GLU:HA	1.92	0.52
3:C:260:ILE:HG22	3:C:261:HIS:N	2.25	0.52
1:A:147:PHE:HE2	1:A:172:ILE:HD13	1.75	0.52
2:B:75:GLN:HA	2:B:75:GLN:NE2	2.25	0.52
3:C:115:TRP:O	3:C:117:PRO:HD3	2.10	0.52
1:A:61:ASN:C	1:A:63:THR:H	2.13	0.52
2:B:97:TYR:O	2:B:100:TYR:HB3	2.10	0.52
1:A:216:SER:CB	1:A:267:LEU:H	2.23	0.51
2:B:155:ASN:O	2:B:159:GLN:HB2	2.10	0.51
2:B:181:LEU:HD23	2:B:181:LEU:O	2.08	0.51
1:A:227:ILE:HG12	1:A:231:ILE:HG12	1.91	0.51
1:A:234:LYS:N	1:A:280:MET:O	2.43	0.51
3:C:134:PHE:CD1	3:C:168:PHE:HB2	2.41	0.51
3:C:98:PRO:HB2	3:C:184:SER:CA	2.41	0.51
2:B:88:ILE:N	2:B:88:ILE:HD12	2.26	0.51
2:B:74:PHE:CD1	2:B:74:PHE:N	2.78	0.51
1:A:85:THR:OG1	1:A:89:LEU:HB2	2.10	0.50
1:A:128:ARG:HD2	1:A:128:ARG:O	2.11	0.50
1:A:130:THR:HG22	1:A:132:LEU:H	1.75	0.50
3:C:133:LYS:HE3	3:C:169:TYR:OH	2.11	0.50
1:A:237:ILE:CB	1:A:250:ILE:HD12	2.41	0.50
3:C:217:VAL:HG11	3:C:273:LEU:HD21	1.93	0.50
2:B:36:ILE:HD12	2:B:36:ILE:N	2.26	0.50
2:B:72:GLY:O	2:B:78:PHE:HA	2.12	0.50
1:A:206:LEU:HA	1:A:221:THR:O	2.11	0.49
1:A:267:LEU:HD22	1:A:273:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:PRO:O	1:A:271:THR:N	2.45	0.49
2:B:137:THR:O	2:B:137:THR:HG22	2.12	0.49
3:C:121:PRO:HB3	3:C:125:THR:HG21	1.93	0.49
1:A:168:TYR:CD1	1:A:195:VAL:HA	2.47	0.49
1:A:102:LEU:HB2	1:A:103:PRO:HD2	1.94	0.49
2:B:81:GLU:O	2:B:85:VAL:HG12	2.12	0.49
1:A:27:VAL:HG23	1:A:27:VAL:O	2.13	0.49
1:A:110:LEU:HD22	1:A:176:VAL:HG23	1.94	0.49
1:A:22:PHE:O	1:A:68:THR:HA	2.13	0.49
1:A:227:ILE:HG12	1:A:227:ILE:O	2.12	0.49
1:A:43:ILE:HD11	1:A:81:CYS:SG	2.53	0.49
1:A:267:LEU:HB3	1:A:273:TYR:CE2	2.47	0.49
2:B:148:LEU:HD23	2:B:148:LEU:C	2.33	0.49
3:C:98:PRO:HD3	3:C:182:LYS:HB3	1.95	0.49
1:A:27:VAL:HG12	1:A:64:ALA:CB	2.41	0.48
2:B:62:LEU:O	2:B:64:LEU:N	2.46	0.48
3:C:108:LEU:HD22	3:C:108:LEU:N	2.28	0.48
3:C:190:GLN:HG2	3:C:191:GLY:N	2.28	0.48
1:A:45:TRP:HD1	1:A:57:TYR:CE2	2.32	0.48
1:A:2:LEU:C	1:A:3:LEU:HD13	2.33	0.48
3:C:129:LEU:HD11	3:C:171:VAL:HB	1.95	0.48
1:A:75:LEU:HB2	1:A:100:SER:H	1.78	0.48
2:B:75:GLN:HE21	2:B:75:GLN:HA	1.78	0.48
3:C:100:LEU:HD12	3:C:101:SER:H	1.77	0.48
1:A:234:LYS:O	1:A:279:CYS:HA	2.14	0.48
2:B:33:LEU:O	2:B:33:LEU:HD13	2.14	0.48
1:A:212:GLU:HB3	3:C:264:TRP:HH2	1.79	0.48
3:C:107:PRO:HD3	3:C:225:TRP:CZ3	2.49	0.48
3:C:209:ALA:C	3:C:211:ASN:H	2.17	0.48
1:A:192:PHE:N	1:A:192:PHE:CD2	2.82	0.48
3:C:102:CYS:SG	3:C:171:VAL:HG21	2.54	0.48
2:B:38:ALA:HA	2:B:41:LYS:HE2	1.96	0.47
1:A:81:CYS:O	1:A:93:VAL:HB	2.14	0.47
2:B:72:GLY:HA2	2:B:77:GLY:O	2.13	0.47
3:C:111:VAL:HB	3:C:159:LEU:HB3	1.96	0.47
3:C:171:VAL:CG2	3:C:187:GLN:HB3	2.43	0.47
1:A:9:ILE:HG22	1:A:10:SER:N	2.29	0.47
1:A:216:SER:HB2	1:A:267:LEU:H	1.79	0.47
3:C:274:ARG:HD3	3:C:287:TRP:CE2	2.49	0.47
1:A:20:SER:O	1:A:72:ILE:HG13	2.13	0.47
1:A:23:THR:HA	1:A:67:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:LEU:O	2:B:94:PHE:HB2	2.15	0.47
3:C:163:GLU:HG3	3:C:230:TYR:OH	2.14	0.47
1:A:220:LEU:HD11	1:A:275:PHE:CD2	2.50	0.47
3:C:99:GLN:NE2	3:C:99:GLN:HA	2.28	0.47
2:B:138:THR:C	2:B:139:PRO:O	2.50	0.47
1:A:192:PHE:N	1:A:192:PHE:HD2	2.13	0.47
1:A:43:ILE:HD12	1:A:82:ASN:O	2.15	0.46
3:C:99:GLN:HA	3:C:99:GLN:HE21	1.79	0.46
1:A:237:ILE:CG2	1:A:250:ILE:HD12	2.45	0.46
2:B:138:THR:O	2:B:138:THR:HG23	2.16	0.46
3:C:108:LEU:HD23	3:C:227:SER:OG	2.15	0.46
3:C:173:MET:HG2	3:C:174:CYS:N	2.30	0.46
2:B:125:PHE:C	2:B:127:GLN:H	2.19	0.46
1:A:112:CYS:HA	1:A:122:CYS:HA	1.96	0.46
3:C:274:ARG:HD3	3:C:287:TRP:CD2	2.50	0.46
2:B:39:LEU:HD23	2:B:39:LEU:N	2.30	0.46
2:B:179:ARG:NH2	3:C:281:GLN:HE22	2.14	0.46
3:C:130:LEU:O	3:C:171:VAL:HA	2.16	0.46
1:A:172:ILE:HD12	1:A:173:GLU:H	1.79	0.46
3:C:110:ASN:HB3	3:C:159:LEU:O	2.15	0.46
1:A:9:ILE:CG2	1:A:10:SER:N	2.79	0.46
1:A:23:THR:HG23	1:A:67:VAL:O	2.16	0.46
1:A:60:ILE:HG22	1:A:61:ASN:N	2.30	0.46
1:A:119:LYS:H	1:A:119:LYS:CD	2.28	0.46
2:B:38:ALA:O	2:B:42:GLU:HB2	2.15	0.46
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.31	0.45
1:A:206:LEU:H	1:A:206:LEU:CD2	2.28	0.45
1:A:212:GLU:O	1:A:214:LEU:N	2.47	0.45
2:B:44:CYS:SG	2:B:50:CYS:C	2.94	0.45
1:A:105:GLU:HB2	1:A:127:GLY:HA3	1.98	0.45
3:C:268:ARG:CA	3:C:294:THR:HG22	2.44	0.45
1:A:9:ILE:HD11	1:A:81:CYS:HB2	1.97	0.45
1:A:206:LEU:HB3	1:A:222:TRP:HB3	1.98	0.45
2:B:100:TYR:OH	2:B:159:GLN:NE2	2.49	0.45
2:B:104:ARG:NH1	2:B:104:ARG:CB	2.80	0.45
2:B:75:GLN:CA	2:B:75:GLN:NE2	2.80	0.45
2:B:138:THR:O	2:B:139:PRO:C	2.55	0.45
1:A:30:GLU:HA	1:A:33:MET:HE3	1.96	0.45
1:A:47:THR:OG1	1:A:50:PHE:HB3	2.16	0.45
1:A:83:ILE:HG23	1:A:93:VAL:HG21	1.99	0.45
2:B:104:ARG:HB3	2:B:104:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:VAL:HG22	3:C:169:TYR:HE1	1.81	0.45
2:B:23:GLU:O	2:B:27:LYS:HB2	2.16	0.45
3:C:231:ARG:HH22	3:C:256:HIS:HE1	1.63	0.45
2:B:43:THR:HG23	2:B:44:CYS:N	2.32	0.44
1:A:12:GLU:O	1:A:96:ILE:HG21	2.16	0.44
1:A:120:MET:O	1:A:162:VAL:HG22	2.18	0.44
1:A:237:ILE:HG12	1:A:277:ILE:HG22	2.00	0.44
2:B:25:ILE:C	2:B:27:LYS:N	2.71	0.44
2:B:87:ILE:HG21	2:B:126:LEU:HD13	1.99	0.44
1:A:172:ILE:HG23	1:A:192:PHE:CD2	2.52	0.44
2:B:25:ILE:C	2:B:27:LYS:H	2.21	0.44
2:B:88:ILE:HD12	2:B:88:ILE:H	1.82	0.44
2:B:36:ILE:H	2:B:36:ILE:CD1	2.31	0.44
2:B:126:LEU:CD2	2:B:181:LEU:HD11	2.47	0.44
3:C:274:ARG:HG2	3:C:287:TRP:CZ3	2.53	0.44
1:A:142:TRP:O	1:A:143:ALA:C	2.55	0.43
3:C:190:GLN:HG2	3:C:191:GLY:H	1.83	0.43
2:B:175:GLN:HG2	3:C:279:PHE:CD2	2.53	0.43
3:C:115:TRP:CE2	3:C:117:PRO:HG3	2.53	0.43
1:A:112:CYS:HB2	1:A:192:PHE:HE1	1.83	0.43
1:A:282:GLU:C	1:A:284:GLY:H	2.21	0.43
1:A:174:VAL:HG22	1:A:175:TRP:N	2.33	0.43
3:C:102:CYS:O	3:C:103:PHE:HB3	2.18	0.43
3:C:104:ARG:O	3:C:195:LEU:HD12	2.18	0.43
3:C:100:LEU:HD21	3:C:171:VAL:HG23	2.01	0.43
1:A:18:LEU:O	1:A:72:ILE:HB	2.18	0.43
1:A:30:GLU:O	1:A:31:LYS:C	2.56	0.43
1:A:100:SER:OG	1:A:101:GLY:N	2.51	0.43
1:A:267:LEU:HD22	1:A:273:TYR:CE2	2.54	0.43
3:C:115:TRP:CH2	3:C:117:PRO:HG3	2.53	0.43
1:A:206:LEU:HG	1:A:295:ALA:HB2	2.01	0.43
1:A:213:GLU:O	1:A:214:LEU:HD22	2.18	0.43
1:A:270:PHE:HD1	1:A:270:PHE:H	1.67	0.43
3:C:236:LEU:HD23	3:C:237:ARG:CA	2.49	0.43
1:A:168:TYR:HD1	1:A:195:VAL:HA	1.82	0.43
2:B:19:LEU:CD2	2:B:24:ARG:HB2	2.48	0.43
2:B:23:GLU:C	2:B:25:ILE:N	2.70	0.43
3:C:100:LEU:HB2	3:C:184:SER:OG	2.19	0.43
3:C:260:ILE:HG22	3:C:261:HIS:H	1.82	0.43
1:A:271:THR:O	1:A:299:THR:HG22	2.18	0.42
3:C:115:TRP:CZ2	3:C:117:PRO:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:TRP:CZ3	3:C:117:PRO:HG3	2.55	0.42
3:C:200:PRO:HD3	3:C:274:ARG:HA	1.99	0.42
1:A:16:VAL:HG12	1:A:17:GLN:N	2.35	0.42
2:B:74:PHE:CD2	3:C:163:GLU:HB3	2.42	0.42
1:A:123:GLU:O	1:A:124:TRP:HB3	2.20	0.42
1:A:291:TRP:HA	1:A:291:TRP:CE3	2.55	0.42
2:B:29:ILE:HG23	2:B:174:LEU:HD22	2.01	0.42
3:C:106:SER:OG	3:C:107:PRO:HD2	2.20	0.42
3:C:235:GLU:HA	3:C:250:MET:HA	2.02	0.42
1:A:124:TRP:CE3	1:A:176:VAL:HG21	2.55	0.42
1:A:10:SER:HA	1:A:11:PRO:C	2.39	0.42
2:B:32:ILE:O	2:B:35:GLY:N	2.51	0.42
2:B:178:LEU:HD23	3:C:279:PHE:CZ	2.30	0.42
3:C:98:PRO:HG2	3:C:183:PHE:HA	2.00	0.42
2:B:136:ILE:HG22	2:B:138:THR:N	2.33	0.41
3:C:264:TRP:CB	3:C:267:LEU:HD12	2.45	0.41
3:C:232:LEU:CD1	3:C:277:GLU:HA	2.50	0.41
3:C:251:VAL:O	3:C:252:LYS:C	2.58	0.41
3:C:277:GLU:O	3:C:279:PHE:N	2.54	0.41
1:A:8:TYR:HA	1:A:94:TYR:CG	2.55	0.41
1:A:102:LEU:HD13	1:A:128:ARG:NE	2.34	0.41
1:A:192:PHE:HD1	1:A:197:LYS:HG3	1.85	0.41
3:C:237:ARG:O	3:C:237:ARG:HG3	2.20	0.41
3:C:277:GLU:O	3:C:278:GLU:C	2.59	0.41
1:A:72:ILE:HG22	1:A:74:SER:O	2.20	0.41
1:A:5:PRO:C	1:A:7:GLY:N	2.73	0.41
1:A:220:LEU:O	1:A:261:SER:HA	2.21	0.41
2:B:88:ILE:H	2:B:88:ILE:CD1	2.34	0.41
1:A:108:LYS:O	1:A:109:ASN:HB2	2.20	0.41
1:A:156:THR:CG2	1:A:159:SER:HB3	2.50	0.41
3:C:278:GLU:HG3	3:C:279:PHE:CE1	2.54	0.41
1:A:137:THR:HG22	1:A:149:ASP:HB3	2.03	0.41
1:A:233:LEU:HD13	1:A:279:CYS:SG	2.61	0.41
3:C:106:SER:OG	3:C:107:PRO:CD	2.69	0.41
3:C:215:LEU:HD11	3:C:269:HIS:CD2	2.56	0.41
1:A:46:LYS:HG2	1:A:51:THR:HA	2.03	0.41
1:A:222:TRP:HE1	1:A:235:TYR:HE2	1.55	0.40
3:C:188:THR:HG22	3:C:189:PHE:N	2.36	0.40
2:B:92:LEU:HD23	2:B:123:ILE:HD13	2.04	0.40
1:A:192:PHE:CD1	1:A:197:LYS:HG3	2.56	0.40
1:A:267:LEU:HB3	1:A:273:TYR:HE2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:TRP:O	3:C:154:LYS:HG3	2.21	0.40
1:A:3:LEU:HD13	1:A:3:LEU:N	2.36	0.40
1:A:222:TRP:CZ3	1:A:261:SER:HA	2.56	0.40
3:C:206:THR:CG2	3:C:207:ALA:N	2.83	0.40
3:C:213:ARG:C	3:C:214:TRP:HD1	2.25	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	296/299 (99%)	232 (78%)	44 (15%)	20 (7%)	1	15
2	B	159/186 (86%)	116 (73%)	34 (21%)	9 (6%)	1	19
3	C	199/201 (99%)	142 (71%)	42 (21%)	15 (8%)	1	13
All	All	654/686 (95%)	490 (75%)	120 (18%)	44 (7%)	1	16

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	30	GLU
1	A	143	ALA
1	A	211	SER
1	A	269	PRO
1	A	270	PHE
2	B	51	GLU
2	B	56	ALA
2	B	63	ASN
3	C	251	VAL
3	C	252	LYS
3	C	253	ASP

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Mol	Chain	Res	Type
3	C	278	GLU
1	A	12	GLU
1	A	31	LYS
1	A	60	ILE
1	A	162	VAL
1	A	298	ILE
2	B	105	PHE
3	C	122	SER
1	A	88	GLN
1	A	157	PRO
1	A	266	ASP
2	B	74	PHE
2	B	172	GLU
3	C	105	LYS
3	C	135	GLN
3	C	231	ARG
3	C	274	ARG
1	A	40	ALA
1	A	49	HIS
1	A	87	GLY
1	A	247	TRP
2	B	24	ARG
2	B	45	ASN
3	C	139	ALA
3	C	181	SER
3	C	265	SER
2	B	65	PRO
3	C	179	VAL
3	C	295	PRO
1	A	251	PRO
3	C	197	PRO
1	A	194	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	275/276 (100%)	259 (94%)	16 (6%)	20	52
2	B	148/167 (89%)	141 (95%)	7 (5%)	26	56
3	C	181/181 (100%)	174 (96%)	7 (4%)	32	60
All	All	604/624 (97%)	574 (95%)	30 (5%)	24	55

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	41	ASN
1	A	56	GLN
1	A	67	VAL
1	A	88	GLN
1	A	128	ARG
1	A	141	GLU
1	A	160	CYS
1	A	188	ASP
1	A	192	PHE
1	A	205	ASN
1	A	210	ASN
1	A	236	ASN
1	A	265	GLN
1	A	269	PRO
1	A	299	THR
2	B	39	LEU
2	B	57	LEU
2	B	74	PHE
2	B	75	GLN
2	B	81	GLU
2	B	94	PHE
2	B	159	GLN
3	C	134	PHE
3	C	155	PHE
3	C	163	GLU
3	C	189	PHE
3	C	210	ARG
3	C	246	PHE
3	C	249	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	115	ASN
1	A	191	ASN
1	A	205	ASN
1	A	236	ASN
1	A	249	GLN
2	B	28	GLN
2	B	75	GLN
2	B	102	GLN
2	B	116	GLN
2	B	124	GLN
2	B	154	GLN
2	B	159	GLN
2	B	175	GLN
3	C	99	GLN
3	C	135	GLN
3	C	147	GLN
3	C	187	GLN
3	C	190	GLN
3	C	196	GLN
3	C	211	ASN
3	C	255	GLN
3	C	281	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 monosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.