Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 02:06 PM EDT

PDB ID	:	5GW0
Title	:	Crystal structure of SNX16 PX-Coiled coil
Authors	:	Xu, J.; Liu, J.
Deposited on	:	2016-09-08
Resolution	:	3.30 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 (i) 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 (1)) were used in the production of this report:

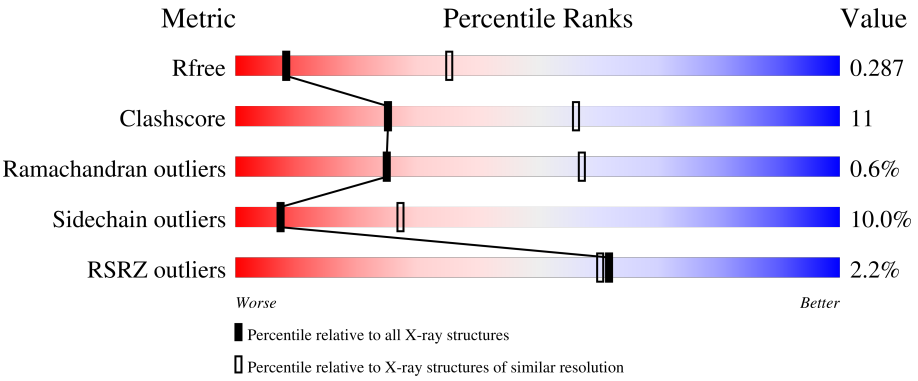
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	179	73% 22%
1	B	179	68% 24% 5%
1	C	179	63% 32%
1	D	179	63% 26% 6% 5%
1	E	179	3% 57% 35%

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Mol	Chain	Length	Quality of chain
1	F	179	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8558 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 Sorting nexin-16.

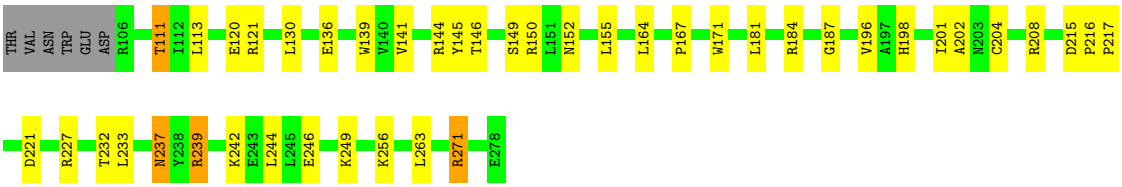
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	Se	0	0	0
			1446	926	246	268	3	3			
1	B	170	Total	C	N	O	S	Se	0	0	0
			1419	911	240	262	3	3			
1	C	173	Total	C	N	O	S	Se	0	0	0
			1446	926	246	268	3	3			
1	D	170	Total	C	N	O	S	Se	0	0	0
			1417	906	242	263	3	3			
1	E	171	Total	C	N	O	S	Se	0	0	0
			1428	915	241	266	3	3			
1	F	168	Total	C	N	O	S	Se	0	0	0
			1402	898	237	261	3	3			

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 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.

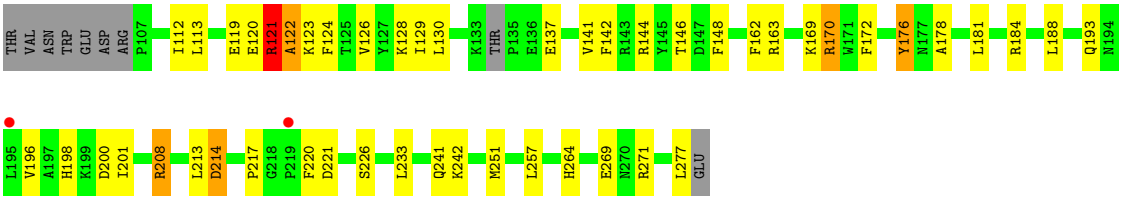
• Molecule 1: Sorting nexin-16

Chain A:



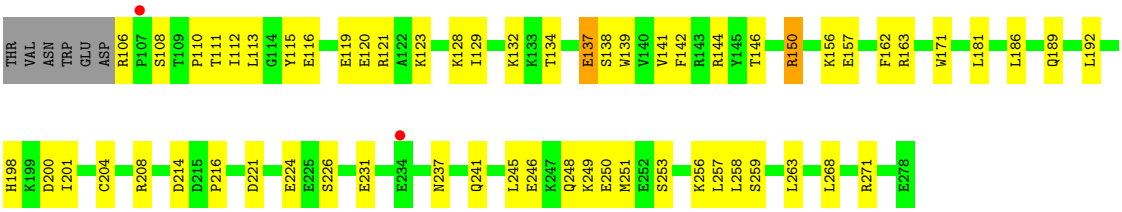
• Molecule 1: Sorting nexin-16

Chain B:



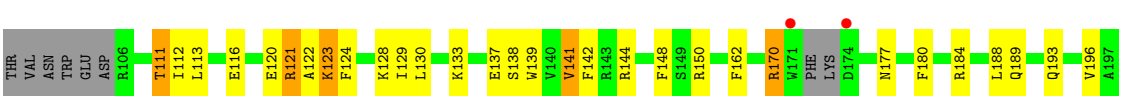
• Molecule 1: Sorting nexin-16

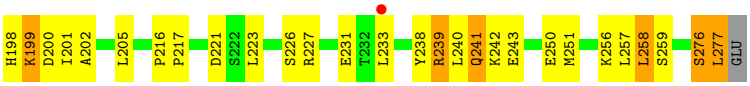
Chain C:



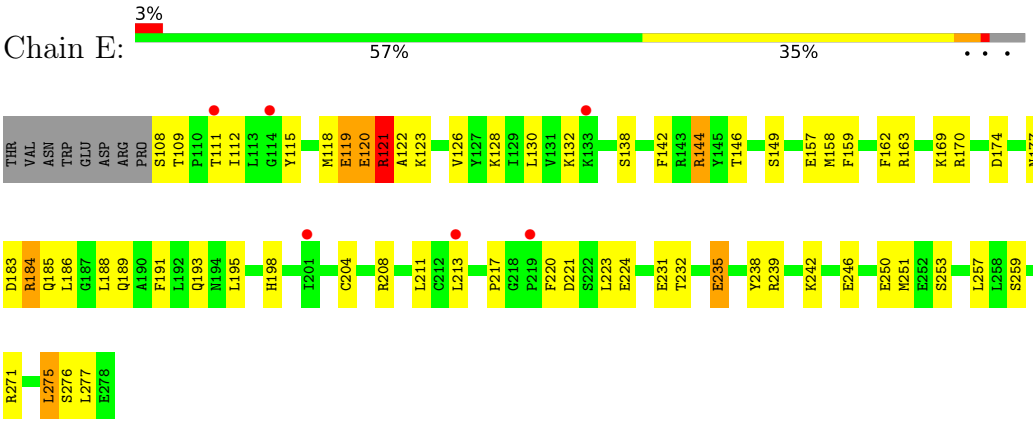
• Molecule 1: Sorting nexin-16

Chain D:

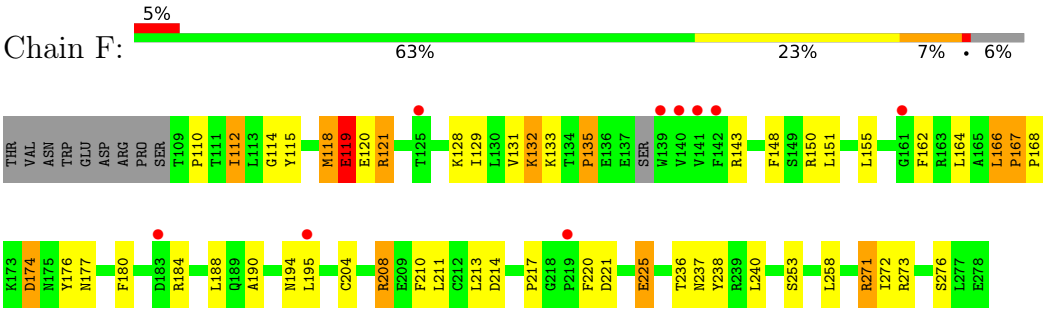




• Molecule 1: Sorting nexin-16



• Molecule 1: Sorting nexin-16



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.38Å 196.78Å 72.96Å 90.00° 111.75° 90.00°	Depositor
Resolution (Å)	19.99 – 3.30 54.45 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-3.30) 98.1 (54.45-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.236 , 0.288 0.236 , 0.287	Depositor DCC
R_{free} test set	1364 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	111.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.056 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8558	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.49	0/1473	0.70	0/1979
1	B	0.43	0/1445	0.66	0/1938
1	C	0.48	0/1473	0.73	0/1979
1	D	0.46	0/1442	0.66	1/1937 (0.1%)
1	E	0.39	0/1454	0.64	1/1953 (0.1%)
1	F	0.35	0/1424	0.68	1/1908 (0.1%)
All	All	0.44	0/8711	0.68	3/11694 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	166	LEU	C-N-CD	-7.86	103.30	120.60
1	E	275	LEU	CA-CB-CG	6.12	129.39	115.30
1	D	122	ALA	N-CA-C	-5.44	96.32	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	E	119	GLU	Peptide
1	F	119	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1446	0	1455	22	0
1	B	1419	0	1430	30	0
1	C	1446	0	1455	36	0
1	D	1417	0	1426	45	0
1	E	1428	0	1435	43	0
1	F	1402	0	1413	33	0
All	All	8558	0	8614	184	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 11.

All (184) 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:F:164:LEU:HD22	1:F:194:ASN:HB3	1.53	0.90
1:C:150:ARG:HH21	1:C:231:GLU:HB2	1.40	0.85
1:D:238:TYR:OH	1:E:198:HIS:NE2	2.13	0.81
1:D:111:THR:HA	1:D:189:GLN:HE22	1.51	0.74
1:E:170:ARG:NH2	1:E:174:ASP:O	2.21	0.73
1:B:126:VAL:HG12	1:B:144:ARG:HG3	1.71	0.71
1:E:231:GLU:OE1	1:E:239:ARG:NH2	2.23	0.71
1:D:238:TYR:HH	1:E:198:HIS:HE2	1.37	0.70
1:F:177:ASN:HB3	1:F:180:PHE:HB3	1.74	0.69
1:E:144:ARG:NH1	1:E:231:GLU:O	2.26	0.69
1:D:142:PHE:HE2	1:D:223:LEU:HD23	1.58	0.67
1:A:120:GLU:O	1:F:121:ARG:HB2	1.95	0.67
1:A:271:ARG:HG2	1:F:272:ILE:HD13	1.77	0.67
1:D:113:LEU:HD11	1:D:130:LEU:HG	1.78	0.66
1:F:190:ALA:O	1:F:194:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:THR:HG21	1:E:193:GLN:HG2	1.79	0.65
1:B:170:ARG:HG2	1:B:184:ARG:HH22	1.62	0.65
1:E:177:ASN:HB3	1:E:180:PHE:HB3	1.80	0.63
1:C:142:PHE:HB2	1:C:226:SER:OG	1.99	0.62
1:A:144:ARG:NH1	1:A:232:THR:HA	2.14	0.62
1:B:214:ASP:OD1	1:B:214:ASP:N	2.28	0.61
1:D:120:GLU:HG3	1:D:124:PHE:HE2	1.64	0.61
1:F:217:PRO:HB2	1:F:221:ASP:HB2	1.81	0.61
1:C:208:ARG:NH1	1:C:214:ASP:OD1	2.34	0.60
1:B:121:ARG:HB2	1:D:121:ARG:HB2	1.84	0.59
1:D:112:ILE:HG12	1:D:129:ILE:HG12	1.82	0.59
1:A:237:ASN:HB2	1:F:237:ASN:OD1	2.03	0.59
1:A:167:PRO:HG3	1:A:187:GLY:HA3	1.84	0.58
1:F:110:PRO:HB3	1:F:131:VAL:HA	1.86	0.58
1:C:198:HIS:CE1	1:C:200:ASP:HB2	2.40	0.57
1:B:129:ILE:HB	1:B:141:VAL:HG23	1.86	0.56
1:F:167:PRO:HB2	1:F:168:PRO:CD	2.34	0.56
1:D:124:PHE:CD1	1:D:144:ARG:HD2	2.41	0.56
1:F:129:ILE:HD11	1:F:148:PHE:HZ	1.69	0.56
1:C:120:GLU:O	1:E:121:ARG:HB2	2.06	0.55
1:F:273:ARG:O	1:F:276:SER:OG	2.20	0.55
1:E:119:GLU:OE2	1:E:121:ARG:NH1	2.37	0.55
1:E:191:PHE:O	1:E:195:LEU:HB2	2.05	0.55
1:E:271:ARG:O	1:E:275:LEU:HD23	2.06	0.55
1:F:112:ILE:HG23	1:F:129:ILE:HG12	1.88	0.55
1:F:170:ARG:HB3	1:F:172:PHE:N	2.21	0.55
1:E:217:PRO:HB2	1:E:221:ASP:HB2	1.89	0.55
1:F:132:LYS:HG3	1:F:135:PRO:HB3	1.90	0.54
1:B:119:GLU:OE2	1:B:121:ARG:HD3	2.08	0.54
1:D:139:TRP:CD2	1:D:216:PRO:HB3	2.43	0.53
1:F:174:ASP:N	1:F:174:ASP:OD1	2.41	0.53
1:C:204:CYS:O	1:C:208:ARG:HG3	2.07	0.53
1:C:139:TRP:CD2	1:C:216:PRO:HB3	2.44	0.53
1:E:250:GLU:O	1:E:253:SER:HB3	2.09	0.53
1:C:134:THR:OG1	1:C:137:GLU:HB2	2.09	0.53
1:B:124:PHE:CD2	1:B:144:ARG:HD2	2.43	0.52
1:D:217:PRO:O	1:D:221:ASP:HB2	2.08	0.52
1:F:167:PRO:HB2	1:F:168:PRO:HD2	1.91	0.52
1:B:198:HIS:HB3	1:B:201:ILE:HB	1.90	0.52
1:C:251:MSE:HB2	1:E:251:MSE:HE2	1.90	0.52
1:F:155:LEU:HD11	1:F:195:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PRO:HG2	1:C:192:LEU:HB3	1.92	0.52
1:C:156:LYS:NZ	1:C:163:ARG:HE	2.08	0.52
1:D:198:HIS:HB3	1:D:201:ILE:HB	1.91	0.52
1:A:121:ARG:HB2	1:F:120:GLU:HB3	1.92	0.51
1:D:142:PHE:HB2	1:D:226:SER:OG	2.11	0.51
1:D:148:PHE:CD2	1:D:188:LEU:HD22	2.45	0.51
1:E:242:LYS:O	1:E:246:GLU:HG2	2.10	0.51
1:A:198:HIS:HB3	1:A:201:ILE:HB	1.92	0.51
1:F:155:LEU:HD13	1:F:164:LEU:HD12	1.93	0.51
1:A:111:THR:HG23	1:A:130:LEU:HB3	1.93	0.51
1:A:204:CYS:O	1:A:208:ARG:HG3	2.11	0.50
1:F:208:ARG:HA	1:F:213:LEU:HD12	1.92	0.50
1:B:162:PHE:HE2	1:B:198:HIS:CD2	2.29	0.50
1:E:130:LEU:HD11	1:E:138:SER:HB2	1.94	0.50
1:C:108:SER:HB2	1:C:132:LYS:O	2.12	0.49
1:F:211:LEU:HB2	1:F:213:LEU:HG	1.94	0.49
1:D:150:ARG:HD3	1:D:239:ARG:HH21	1.77	0.49
1:B:257:LEU:HD23	1:D:258:LEU:HD11	1.94	0.49
1:C:245:LEU:HD11	1:C:249:LYS:HE3	1.94	0.49
1:D:239:ARG:HD3	1:D:243:GLU:OE2	2.13	0.48
1:F:143:ARG:NH2	1:F:225:GLU:OE2	2.46	0.48
1:C:112:ILE:H	1:C:189:GLN:HE22	1.60	0.48
1:D:196:VAL:HA	1:D:202:ALA:HB2	1.95	0.48
1:F:118:MSE:C	1:F:119:GLU:HG2	2.34	0.48
1:B:208:ARG:HD2	1:B:213:LEU:HB2	1.94	0.48
1:C:268:LEU:HB2	1:E:268:LEU:HD13	1.94	0.48
1:A:171:TRP:CD1	1:F:238:TYR:HB2	2.49	0.48
1:B:198:HIS:CE1	1:B:200:ASP:HB2	2.48	0.48
1:C:198:HIS:ND1	1:C:201:ILE:HG12	2.29	0.48
1:D:123:LYS:H	1:D:123:LYS:HD2	1.79	0.47
1:D:233:LEU:HD12	1:D:233:LEU:H	1.79	0.47
1:A:139:TRP:CE2	1:A:216:PRO:HB3	2.48	0.47
1:D:198:HIS:HE1	1:D:200:ASP:HB2	1.80	0.47
1:D:256:LYS:O	1:D:259:SER:HB3	2.15	0.47
1:A:217:PRO:O	1:A:221:ASP:HB2	2.14	0.47
1:B:251:MSE:SE	1:D:250:GLU:HB3	2.64	0.47
1:F:133:LYS:HE2	1:F:133:LYS:HB3	1.63	0.47
1:E:162:PHE:HE2	1:E:198:HIS:CD2	2.33	0.47
1:E:204:CYS:O	1:E:208:ARG:HG3	2.15	0.47
1:D:130:LEU:HD23	1:D:130:LEU:HA	1.62	0.47
1:D:223:LEU:O	1:D:227:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PRO:HB2	1:B:221:ASP:HB2	1.97	0.47
1:C:128:LYS:HG3	1:C:142:PHE:CE1	2.49	0.47
1:B:169:LYS:NZ	1:D:241:GLN:OE1	2.32	0.47
1:F:236:THR:O	1:F:240:LEU:HG	2.14	0.46
1:A:155:LEU:HD13	1:A:164:LEU:HD13	1.97	0.46
1:D:198:HIS:CE1	1:D:200:ASP:HB2	2.51	0.46
1:B:148:PHE:CE2	1:B:188:LEU:HD13	2.50	0.46
1:B:120:GLU:OE1	1:D:121:ARG:HB3	2.15	0.45
1:C:132:LYS:HB3	1:C:138:SER:HB3	1.98	0.45
1:B:123:LYS:O	1:B:176:TYR:OH	2.34	0.45
1:B:241:GLN:HE22	1:D:240:LEU:HD21	1.81	0.45
1:D:116:GLU:HG3	1:D:128:LYS:HE2	1.99	0.45
1:E:211:LEU:HB2	1:E:213:LEU:HG	1.98	0.45
1:B:178:ALA:HA	1:B:181:LEU:HB2	1.99	0.45
1:A:113:LEU:HD11	1:A:130:LEU:HB2	1.98	0.45
1:F:204:CYS:O	1:F:208:ARG:HG2	2.17	0.45
1:D:170:ARG:HG3	1:D:184:ARG:HH22	1.81	0.45
1:A:196:VAL:HA	1:A:202:ALA:HB2	1.99	0.44
1:C:139:TRP:CG	1:C:216:PRO:HB3	2.53	0.44
1:D:242:LYS:HA	1:D:242:LYS:HD2	1.78	0.44
1:F:114:GLY:H	1:F:128:LYS:HG3	1.83	0.44
1:B:112:ILE:HA	1:B:129:ILE:HA	1.98	0.44
1:C:250:GLU:O	1:C:253:SER:HB3	2.17	0.44
1:D:129:ILE:HB	1:D:141:VAL:HG23	1.99	0.44
1:C:132:LYS:HB3	1:C:138:SER:CB	2.48	0.44
1:D:205:LEU:HD13	1:E:183:ASP:CG	2.38	0.44
1:C:181:LEU:HD23	1:C:181:LEU:HA	1.86	0.44
1:D:112:ILE:HA	1:D:129:ILE:HA	1.99	0.44
1:C:221:ASP:O	1:C:224:GLU:HB3	2.18	0.44
1:D:133:LYS:O	1:D:137:GLU:HB3	2.18	0.44
1:F:164:LEU:HD22	1:F:194:ASN:CB	2.37	0.43
1:B:121:ARG:HG3	1:D:121:ARG:HH11	1.83	0.43
1:C:116:GLU:OE1	1:C:116:GLU:HA	2.18	0.43
1:C:241:GLN:OE1	1:E:169:LYS:HE3	2.18	0.43
1:E:182:GLU:O	1:E:185:GLN:HB3	2.18	0.43
1:E:108:SER:HB3	1:E:132:LYS:O	2.18	0.43
1:E:120:GLU:O	1:E:122:ALA:N	2.52	0.43
1:E:128:LYS:HG2	1:E:142:PHE:CE2	2.54	0.43
1:A:146:THR:O	1:A:149:SER:HB3	2.18	0.43
1:B:113:LEU:HD11	1:B:130:LEU:HB2	2.01	0.43
1:B:119:GLU:HG2	1:B:123:LYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TYR:HA	1:B:181:LEU:CD1	2.49	0.43
1:F:208:ARG:O	1:F:213:LEU:N	2.46	0.43
1:E:126:VAL:HG21	1:E:142:PHE:HB3	2.01	0.42
1:E:119:GLU:OE1	1:E:123:LYS:HE3	2.19	0.42
1:E:181:LEU:HD23	1:E:181:LEU:HA	1.80	0.42
1:C:121:ARG:O	1:E:120:GLU:HB2	2.20	0.42
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.74	0.42
1:A:246:GLU:O	1:A:249:LYS:HB2	2.20	0.42
1:B:142:PHE:HB2	1:B:226:SER:HB2	2.01	0.42
1:B:148:PHE:CD2	1:B:188:LEU:HD22	2.55	0.42
1:E:158:MSE:HB2	1:E:159:PHE:CD1	2.55	0.42
1:B:193:GLN:O	1:B:196:VAL:HG12	2.20	0.42
1:D:150:ARG:HH22	1:D:231:GLU:HB3	1.84	0.42
1:D:251:MSE:HE2	1:D:251:MSE:HB3	1.99	0.42
1:A:150:ARG:HD3	1:A:239:ARG:NH1	2.34	0.41
1:B:122:ALA:CB	1:D:233:LEU:HD13	2.49	0.41
1:D:162:PHE:CE2	1:D:198:HIS:CD2	3.09	0.41
1:D:199:LYS:HB3	1:D:199:LYS:HE2	1.74	0.41
1:C:198:HIS:HE1	1:C:200:ASP:HB2	1.85	0.41
1:D:276:SER:OG	1:D:277:LEU:HD23	2.20	0.41
1:E:118:MSE:HE1	1:E:223:LEU:HD23	2.03	0.41
1:E:144:ARG:H	1:E:144:ARG:HG2	1.70	0.41
1:B:242:LYS:HD2	1:B:242:LYS:HA	1.81	0.41
1:C:113:LEU:HD12	1:C:128:LYS:HD3	2.02	0.41
1:C:129:ILE:HD12	1:C:141:VAL:HG23	2.02	0.41
1:C:150:ARG:HH11	1:C:150:ARG:HB3	1.85	0.41
1:C:171:TRP:CD1	1:E:238:TYR:CD1	3.09	0.41
1:C:258:LEU:HD21	1:E:257:LEU:HD23	2.03	0.41
1:E:235:GLU:H	1:E:235:GLU:HG2	1.47	0.41
1:A:121:ARG:CB	1:F:120:GLU:HB3	2.51	0.41
1:A:145:TYR:CD1	1:A:184:ARG:HD2	2.56	0.41
1:C:271:ARG:HD2	1:C:271:ARG:HA	1.89	0.41
1:C:171:TRP:CD1	1:E:238:TYR:HD1	2.39	0.41
1:E:146:THR:O	1:E:149:SER:HB3	2.21	0.41
1:E:208:ARG:HA	1:E:213:LEU:HD12	2.03	0.41
1:F:271:ARG:HA	1:F:271:ARG:HD2	1.73	0.41
1:C:144:ARG:NH1	1:C:231:GLU:O	2.54	0.41
1:D:139:TRP:CE2	1:D:216:PRO:HB3	2.56	0.40
1:E:115:TYR:CE1	1:E:181:LEU:HD13	2.57	0.40
1:A:120:GLU:O	1:A:121:ARG:HB2	2.21	0.40
1:C:115:TYR:CE2	1:C:181:LEU:HD13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:LEU:HD22	1:F:210:PHE:CD2	2.56	0.40
1:D:177:ASN:HB3	1:D:180:PHE:HB3	2.03	0.40
1:E:112:ILE:HG22	1:E:189:GLN:CD	2.42	0.40
1:E:221:ASP:O	1:E:224:GLU:HB3	2.21	0.40
1:E:184:ARG:O	1:E:188:LEU:HG	2.22	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	171/179 (96%)	167 (98%)	4 (2%)	0	100 100
1	B	166/179 (93%)	157 (95%)	8 (5%)	1 (1%)	25 57
1	C	171/179 (96%)	167 (98%)	4 (2%)	0	100 100
1	D	166/179 (93%)	160 (96%)	6 (4%)	0	100 100
1	E	169/179 (94%)	162 (96%)	6 (4%)	1 (1%)	25 57
1	F	162/179 (90%)	151 (93%)	7 (4%)	4 (2%)	5 27
All	All	1005/1074 (94%)	964 (96%)	35 (4%)	6 (1%)	25 57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	121	ARG
1	F	121	ARG
1	B	122	ALA
1	F	135	PRO
1	F	166	LEU
1	F	167	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	161/164 (98%)	147 (91%)	14 (9%)	10	34
1	B	158/164 (96%)	142 (90%)	16 (10%)	7	27
1	C	161/164 (98%)	144 (89%)	17 (11%)	6	25
1	D	158/164 (96%)	144 (91%)	14 (9%)	9	32
1	E	159/164 (97%)	144 (91%)	15 (9%)	8	30
1	F	156/164 (95%)	137 (88%)	19 (12%)	5	20
All	All	953/984 (97%)	858 (90%)	95 (10%)	7	27

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	THR
1	A	136	GLU
1	A	141	VAL
1	A	152	ASN
1	A	215	ASP
1	A	227	ARG
1	A	233	LEU
1	A	237	ASN
1	A	239	ARG
1	A	242	LYS
1	A	244	LEU
1	A	256	LYS
1	A	263	LEU
1	A	271	ARG
1	B	121	ARG
1	B	128	LYS
1	B	137	GLU
1	B	146	THR
1	B	163	ARG
1	B	170	ARG
1	B	172	PHE
1	B	176	TYR

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Mol	Chain	Res	Type
1	B	208	ARG
1	B	214	ASP
1	B	220	PHE
1	B	233	LEU
1	B	264	HIS
1	B	269	GLU
1	B	271	ARG
1	B	277	LEU
1	C	106	ARG
1	C	111	THR
1	C	119	GLU
1	C	123	LYS
1	C	137	GLU
1	C	146	THR
1	C	150	ARG
1	C	157	GLU
1	C	162	PHE
1	C	186	LEU
1	C	237	ASN
1	C	246	GLU
1	C	248	GLN
1	C	256	LYS
1	C	257	LEU
1	C	259	SER
1	C	263	LEU
1	D	111	THR
1	D	121	ARG
1	D	123	LYS
1	D	138	SER
1	D	141	VAL
1	D	170	ARG
1	D	193	GLN
1	D	199	LYS
1	D	239	ARG
1	D	241	GLN
1	D	257	LEU
1	D	258	LEU
1	D	276	SER
1	D	277	LEU
1	E	111	THR
1	E	120	GLU
1	E	121	ARG

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Mol	Chain	Res	Type
1	E	144	ARG
1	E	157	GLU
1	E	163	ARG
1	E	184	ARG
1	E	186	LEU
1	E	220	PHE
1	E	232	THR
1	E	235	GLU
1	E	259	SER
1	E	262	GLN
1	E	276	SER
1	E	277	LEU
1	F	112	ILE
1	F	115	TYR
1	F	118	MSE
1	F	119	GLU
1	F	132	LYS
1	F	150	ARG
1	F	162	PHE
1	F	172	PHE
1	F	174	ASP
1	F	176	TYR
1	F	184	ARG
1	F	188	LEU
1	F	208	ARG
1	F	214	ASP
1	F	220	PHE
1	F	225	GLU
1	F	253	SER
1	F	258	LEU
1	F	271	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	194	ASN

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 monosaccharides 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	170/179 (94%)	0.11	0 100 100	42, 75, 111, 129	0
1	B	167/179 (93%)	0.17	2 (1%) 79 78	59, 87, 142, 163	0
1	C	170/179 (94%)	0.16	2 (1%) 79 78	35, 68, 113, 131	0
1	D	167/179 (93%)	0.05	3 (1%) 68 67	45, 81, 120, 168	0
1	E	168/179 (93%)	0.24	6 (3%) 42 40	65, 113, 155, 169	0
1	F	165/179 (92%)	0.18	9 (5%) 25 23	57, 133, 183, 190	0
All	All	1007/1074 (93%)	0.15	22 (2%) 62 60	35, 87, 162, 190	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	219	PRO	7.0
1	F	195	LEU	4.6
1	C	107	PRO	3.9
1	D	171	TRP	3.1
1	B	219	PRO	3.1
1	E	213	LEU	3.0
1	E	133	LYS	2.9
1	F	140	VAL	2.7
1	D	174	ASP	2.6
1	E	201	ILE	2.5
1	D	233	LEU	2.5
1	C	234	GLU	2.4
1	F	141	VAL	2.4
1	F	161	GLY	2.3
1	F	139	TRP	2.3
1	F	142	PHE	2.3
1	F	183	ASP	2.3
1	B	195	LEU	2.3
1	F	125	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	114	GLY	2.2
1	F	219	PRO	2.1
1	E	111	THR	2.1

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 monosaccharides 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.