



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:15 PM EDT

PDB ID : 5GW1
Title : Crystal structure of SNX16 PX-Coiled coil in space group P212121
Authors : Xu, J.; Liu, J.
Deposited on : 2016-09-08
Resolution : 3.35 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
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

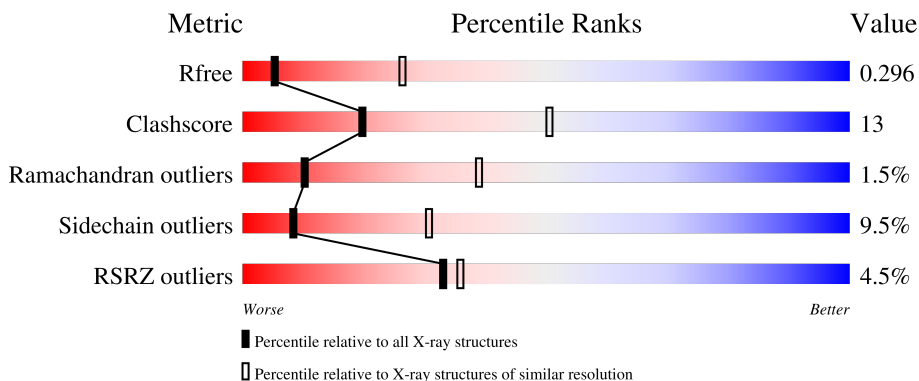
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.



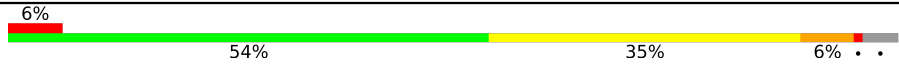


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 $\leq 5\%$. 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	 71% 24% . .
1	B	179	 8% 58% 36% . .
1	C	179	 4% 64% 30% . .
1	D	179	 2% 64% 28% . . .
1	E	179	 % 72% 23% . .

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Mol	Chain	Length	Quality of chain
1	F	179	
1	G	179	
1	H	179	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11563 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.

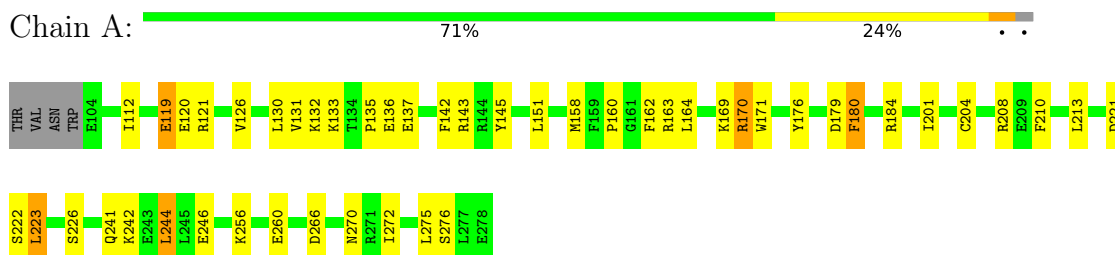
- Molecule 1 is a protein called Sorting nexin-16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	175	1463	935	248	274	3	3	0	0	0
1	B	173	1445	925	246	268	3	3	0	0	0
1	C	176	1477	946	250	275	3	3	0	0	0
1	D	172	1437	921	245	265	3	3	0	0	0
1	E	176	1477	946	250	275	3	3	0	0	0
1	F	171	1431	916	244	265	3	3	0	0	0
1	G	165	1387	892	235	254	3	3	0	0	0
1	H	173	1446	926	246	268	3	3	0	0	0

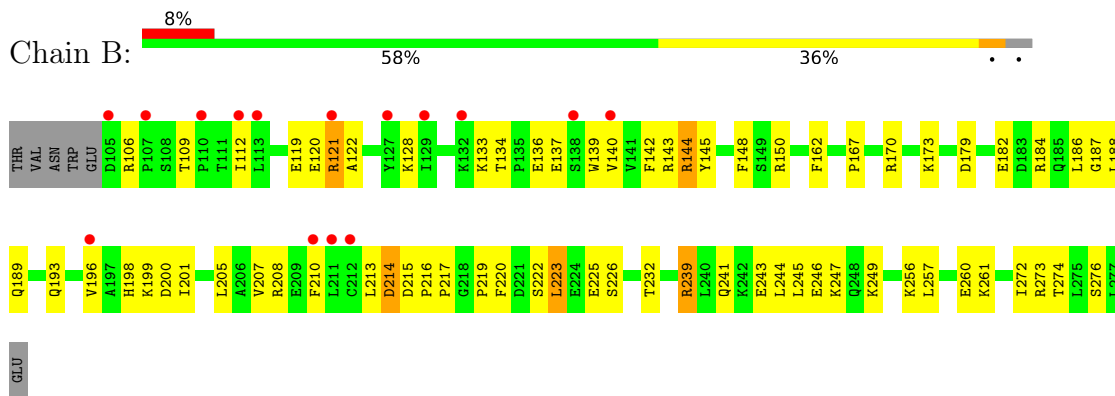
3 Residue-property plots [i](#)

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 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.

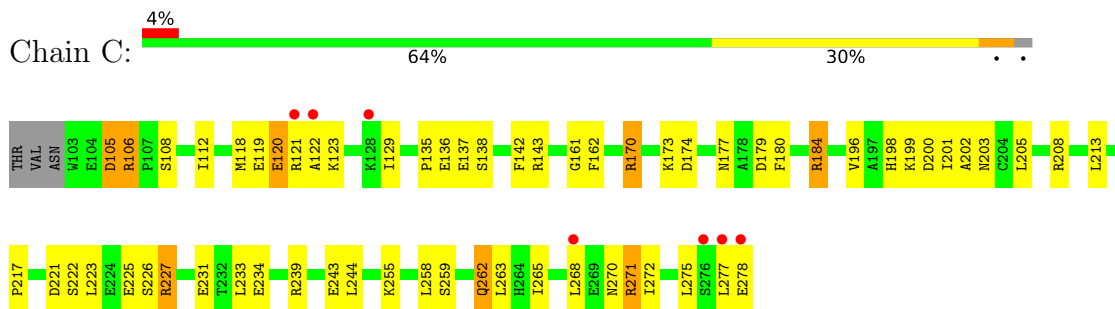
- Molecule 1: Sorting nexin-16



- Molecule 1: Sorting nexin-16

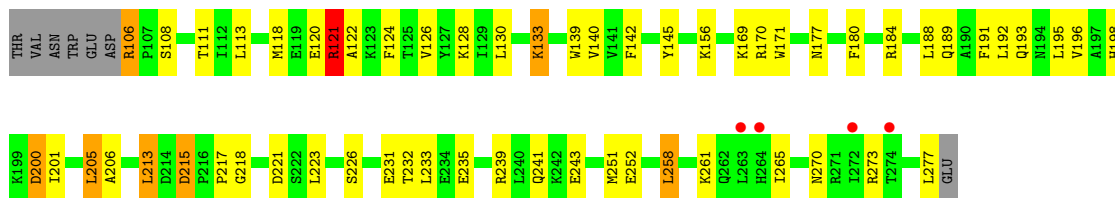


- Molecule 1: Sorting nexin-16

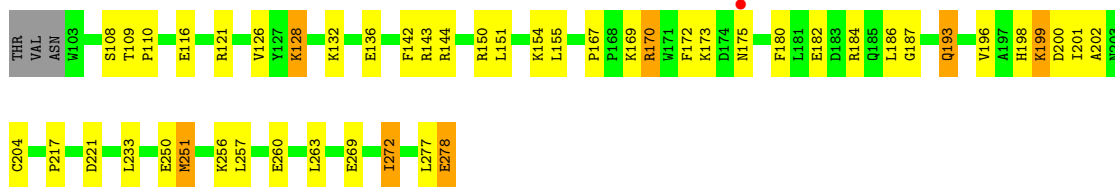


- Molecule 1: Sorting nexin-16

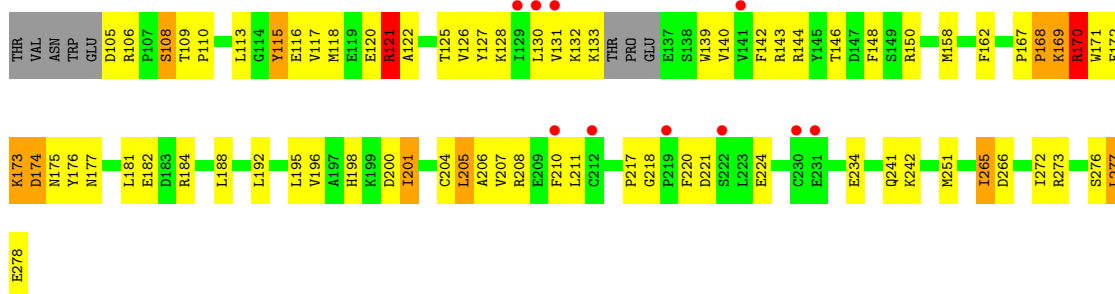




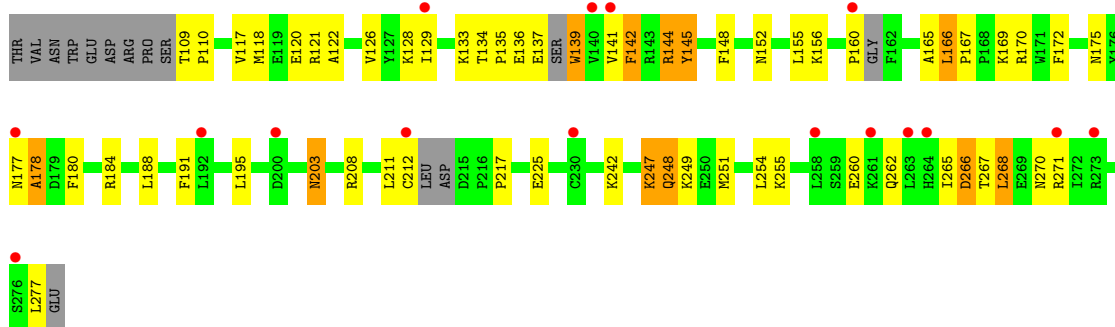
• Molecule 1: Sorting nexin-16



• Molecule 1: Sorting nexin-16

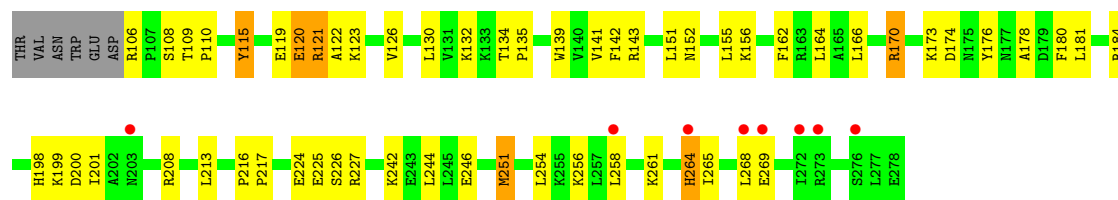


• Molecule 1: Sorting nexin-16



• Molecule 1: Sorting nexin-16





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.67Å 133.06Å 215.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.35 56.60 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.35) 99.6 (56.60-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.257 , 0.286 0.270 , 0.296	Depositor DCC
R_{free} test set	1578 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	104.1	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.46	0/1490	0.71	0/2002
1	B	0.39	0/1472	0.65	1/1978 (0.1%)
1	C	0.41	0/1506	0.66	0/2025
1	D	0.41	0/1464	0.67	0/1967
1	E	0.45	0/1506	0.70	0/2025
1	F	0.39	0/1456	0.68	0/1953
1	G	0.41	0/1410	0.76	2/1889 (0.1%)
1	H	0.50	0/1473	0.74	0/1979
All	All	0.43	0/11777	0.70	3/15818 (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	A	0	2
1	B	0	1
1	G	0	1
1	H	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	122	ALA	N-CA-C	-6.10	94.53	111.00
1	G	195	LEU	N-CA-C	5.46	125.73	111.00
1	B	239	ARG	NE-CZ-NH1	-5.12	117.74	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLU	Peptide
1	A	176	TYR	Peptide
1	B	119	GLU	Peptide
1	G	178	ALA	Peptide
1	H	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	1463	0	1465	33	0
1	B	1445	0	1453	46	0
1	C	1477	0	1475	40	0
1	D	1437	0	1449	36	0
1	E	1477	0	1475	26	0
1	F	1431	0	1438	53	0
1	G	1387	0	1398	42	0
1	H	1446	0	1455	41	0
All	All	11563	0	11608	295	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 13.

All (295) 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:173:LYS:HB2	1:G:160:PRO:HD3	1.42	1.01
1:B:217:PRO:HG3	1:B:225:GLU:HG2	1.57	0.87
1:F:172:PHE:O	1:F:175:ASN:ND2	2.14	0.80
1:A:169:LYS:HG3	1:A:171:TRP:H	1.47	0.80
1:F:148:PHE:HD2	1:F:188:LEU:HD22	1.50	0.77
1:F:218:GLY:H	1:F:221:ASP:HB3	1.51	0.76
1:F:167:PRO:HG2	1:F:184:ARG:HA	1.69	0.74
1:C:123:LYS:HG3	1:D:121:ARG:HH21	1.52	0.73
1:H:139:TRP:CD2	1:H:216:PRO:HB3	2.23	0.73
1:B:148:PHE:HD2	1:B:188:LEU:HD22	1.53	0.73
1:G:167:PRO:O	1:G:169:LYS:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:O	1:A:184:ARG:N	2.20	0.71
1:H:173:LYS:HG2	1:H:174:ASP:H	1.56	0.71
1:G:267:THR:OG1	1:G:271:ARG:NH2	2.24	0.71
1:D:177:ASN:HB2	1:D:180:PHE:HB2	1.72	0.69
1:G:129:ILE:HG21	1:G:211:LEU:HD21	1.74	0.68
1:C:119:GLU:HA	1:C:122:ALA:O	1.93	0.68
1:C:162:PHE:CE1	1:C:201:ILE:HD11	2.29	0.67
1:H:162:PHE:CE1	1:H:201:ILE:HD11	2.29	0.67
1:A:120:GLU:C	1:B:121:ARG:HB2	2.16	0.66
1:B:222:SER:O	1:B:225:GLU:HG3	1.95	0.66
1:C:239:ARG:NH1	1:C:243:GLU:OE2	2.29	0.66
1:C:120:GLU:OE2	1:C:121:ARG:NH1	2.29	0.66
1:G:170:ARG:NH1	1:G:175:ASN:OD1	2.25	0.66
1:A:142:PHE:O	1:A:143:ARG:NH1	2.28	0.65
1:E:198:HIS:ND1	1:E:198:HIS:O	2.29	0.65
1:B:208:ARG:HH11	1:B:213:LEU:HD22	1.61	0.65
1:H:134:THR:HB	1:H:135:PRO:HD2	1.79	0.65
1:A:221:ASP:O	1:A:223:LEU:N	2.28	0.64
1:B:208:ARG:NH1	1:B:214:ASP:OD1	2.31	0.64
1:B:136:GLU:HG2	1:B:137:GLU:H	1.62	0.63
1:G:262:GLN:HA	1:G:265:ILE:HG12	1.78	0.63
1:G:133:LYS:HG3	1:G:134:THR:H	1.64	0.63
1:C:271:ARG:O	1:C:271:ARG:NH1	2.32	0.63
1:E:126:VAL:HG12	1:E:144:ARG:HG2	1.81	0.63
1:A:120:GLU:O	1:B:121:ARG:HB2	1.99	0.63
1:F:113:LEU:HD12	1:F:128:LYS:HB3	1.81	0.63
1:F:118:MSE:HE3	1:F:126:VAL:HG11	1.81	0.62
1:F:205:LEU:O	1:F:208:ARG:N	2.33	0.62
1:C:142:PHE:O	1:C:143:ARG:NH1	2.27	0.62
1:F:198:HIS:HE1	1:F:200:ASP:HB2	1.64	0.61
1:G:120:GLU:C	1:H:121:ARG:HB2	2.20	0.61
1:C:170:ARG:HG3	1:C:180:PHE:CE1	2.35	0.61
1:B:128:LYS:HE3	1:B:140:VAL:HG11	1.82	0.61
1:B:150:ARG:HD3	1:B:239:ARG:HH12	1.65	0.60
1:D:126:VAL:HG21	1:D:142:PHE:HB3	1.83	0.60
1:B:133:LYS:HG3	1:B:134:THR:H	1.66	0.60
1:B:144:ARG:HH21	1:B:232:THR:HA	1.67	0.59
1:F:169:LYS:HE2	1:F:175:ASN:H	1.67	0.59
1:B:189:GLN:O	1:B:193:GLN:HG2	2.02	0.59
1:C:170:ARG:HD3	1:C:173:LYS:HB2	1.85	0.59
1:B:148:PHE:CE1	1:B:210:PHE:HZ	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:HB3	1:A:121:ARG:H	1.69	0.58
1:C:208:ARG:HG2	1:C:213:LEU:HD12	1.85	0.58
1:F:198:HIS:CE1	1:F:200:ASP:HB2	2.38	0.58
1:F:108:SER:OG	1:F:109:THR:N	2.32	0.58
1:C:105:ASP:HB3	1:C:203:ASN:HD21	1.68	0.58
1:D:120:GLU:HG2	1:D:124:PHE:CE1	2.39	0.57
1:C:162:PHE:HE1	1:C:201:ILE:HD11	1.69	0.57
1:H:139:TRP:CE3	1:H:216:PRO:HB3	2.38	0.57
1:G:203:ASN:HB3	1:G:208:ARG:CZ	2.35	0.57
1:G:265:ILE:HD12	1:H:264:HIS:ND1	2.20	0.56
1:B:145:TYR:OH	1:B:167:PRO:O	2.24	0.56
1:C:198:HIS:O	1:C:198:HIS:ND1	2.39	0.56
1:G:251:MSE:HE3	1:H:254:LEU:HD22	1.86	0.56
1:E:109:THR:OG1	1:E:193:GLN:NE2	2.39	0.56
1:G:170:ARG:HG2	1:G:172:PHE:H	1.71	0.56
1:H:120:GLU:O	1:H:122:ALA:N	2.38	0.55
1:D:170:ARG:HG2	1:D:184:ARG:HH21	1.72	0.55
1:C:233:LEU:HD12	1:C:233:LEU:H	1.72	0.55
1:F:142:PHE:O	1:F:143:ARG:NH1	2.36	0.55
1:D:215:ASP:N	1:D:215:ASP:OD1	2.38	0.54
1:H:143:ARG:NH2	1:H:225:GLU:OE2	2.40	0.54
1:H:265:ILE:O	1:H:269:GLU:HB2	2.07	0.54
1:B:142:PHE:O	1:B:143:ARG:NH1	2.40	0.54
1:G:148:PHE:CD2	1:G:188:LEU:HD22	2.43	0.54
1:E:272:ILE:HD13	1:F:272:ILE:HG12	1.90	0.54
1:H:141:VAL:HB	1:H:143:ARG:NH1	2.23	0.54
1:A:133:LYS:HD3	1:A:137:GLU:OE1	2.07	0.54
1:A:201:ILE:O	1:A:204:CYS:HB3	2.08	0.54
1:C:272:ILE:HA	1:C:275:LEU:HD12	1.90	0.54
1:C:135:PRO:O	1:C:137:GLU:N	2.39	0.53
1:H:120:GLU:C	1:H:122:ALA:H	2.10	0.53
1:H:123:LYS:O	1:H:176:TYR:OH	2.26	0.53
1:B:144:ARG:NH2	1:B:232:THR:HA	2.23	0.53
1:D:192:LEU:HD23	1:D:195:LEU:HD12	1.89	0.53
1:B:142:PHE:CE2	1:B:222:SER:HB2	2.44	0.53
1:C:199:LYS:O	1:C:202:ALA:N	2.41	0.53
1:A:180:PHE:HZ	1:A:184:ARG:HH21	1.55	0.53
1:F:218:GLY:H	1:F:221:ASP:CB	2.19	0.53
1:F:277:LEU:O	1:F:278:GLU:HB3	2.08	0.53
1:A:160:PRO:HA	1:A:163:ARG:HH21	1.73	0.52
1:F:110:PRO:HG3	1:F:131:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASP:OD1	1:D:200:ASP:N	2.28	0.52
1:E:172:PHE:O	1:E:173:LYS:HB2	2.10	0.52
1:B:120:GLU:C	1:B:122:ALA:H	2.14	0.51
1:G:170:ARG:NE	1:G:172:PHE:O	2.43	0.51
1:B:148:PHE:CD2	1:B:188:LEU:HD22	2.41	0.51
1:B:109:THR:HA	1:B:196:VAL:HG21	1.93	0.51
1:C:217:PRO:HB2	1:C:221:ASP:HB3	1.93	0.51
1:F:169:LYS:HA	1:F:172:PHE:CZ	2.46	0.51
1:B:150:ARG:CD	1:B:239:ARG:HH12	2.23	0.51
1:D:223:LEU:O	1:D:226:SER:HB3	2.10	0.51
1:C:222:SER:O	1:C:225:GLU:HB3	2.11	0.51
1:H:170:ARG:HG3	1:H:180:PHE:CE1	2.46	0.51
1:H:173:LYS:HG2	1:H:174:ASP:N	2.24	0.50
1:E:116:GLU:HB2	1:E:128:LYS:HE2	1.93	0.50
1:G:134:THR:HG22	1:G:135:PRO:HD2	1.94	0.50
1:B:256:LYS:O	1:B:260:GLU:HG3	2.11	0.50
1:H:208:ARG:HG2	1:H:213:LEU:HD12	1.92	0.50
1:A:162:PHE:HE1	1:A:164:LEU:HD21	1.76	0.50
1:A:169:LYS:HD2	1:A:170:ARG:HH11	1.76	0.50
1:B:120:GLU:O	1:B:122:ALA:N	2.44	0.50
1:H:152:ASN:O	1:H:156:LYS:HG3	2.11	0.50
1:B:243:GLU:O	1:B:247:LYS:HG2	2.12	0.50
1:B:198:HIS:ND1	1:B:199:LYS:O	2.43	0.50
1:D:145:TYR:OH	1:D:169:LYS:HG3	2.12	0.50
1:G:268:LEU:CD1	1:H:268:LEU:HD13	2.42	0.50
1:A:151:LEU:HD22	1:A:210:PHE:CG	2.47	0.49
1:F:146:THR:HG23	1:F:171:TRP:CZ2	2.47	0.49
1:D:120:GLU:C	1:D:122:ALA:H	2.15	0.49
1:F:117:VAL:HG22	1:F:125:THR:HG22	1.94	0.49
1:D:133:LYS:HE3	1:D:213:LEU:HD11	1.93	0.49
1:A:136:GLU:N	1:A:136:GLU:OE1	2.45	0.49
1:G:268:LEU:HD11	1:H:268:LEU:HD13	1.95	0.49
1:E:251:MSE:SE	1:F:251:MSE:HB3	2.62	0.49
1:C:170:ARG:HG2	1:C:170:ARG:HH11	1.77	0.49
1:G:128:LYS:HG2	1:G:142:PHE:HE1	1.76	0.49
1:C:170:ARG:HD2	1:C:174:ASP:O	2.13	0.48
1:E:167:PRO:HD3	1:E:187:GLY:HA3	1.94	0.48
1:B:148:PHE:HE2	1:B:188:LEU:HB3	1.78	0.48
1:G:254:LEU:HB3	1:H:254:LEU:HD21	1.94	0.48
1:H:224:GLU:OE2	1:H:227:ARG:NH2	2.45	0.48
1:D:189:GLN:O	1:D:193:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:LEU:HD12	1:E:233:LEU:H	1.77	0.48
1:F:207:VAL:O	1:F:211:LEU:HG	2.13	0.48
1:G:120:GLU:O	1:H:121:ARG:HB2	2.13	0.48
1:A:256:LYS:HG2	1:A:260:GLU:OE2	2.13	0.48
1:F:169:LYS:HE2	1:F:174:ASP:HB2	1.96	0.48
1:B:184:ARG:O	1:B:188:LEU:HG	2.13	0.48
1:H:130:LEU:HD21	1:H:132:LYS:HE3	1.94	0.48
1:D:106:ARG:O	1:D:108:SER:N	2.45	0.48
1:G:251:MSE:HE2	1:G:255:LYS:HE3	1.94	0.48
1:A:126:VAL:HG11	1:A:142:PHE:HB3	1.95	0.48
1:D:231:GLU:HA	1:D:235:GLU:OE1	2.14	0.48
1:A:221:ASP:C	1:A:223:LEU:H	2.15	0.48
1:G:121:ARG:HB2	1:H:120:GLU:C	2.34	0.48
1:B:182:GLU:O	1:B:186:LEU:HG	2.14	0.47
1:E:199:LYS:HE2	1:E:199:LYS:N	2.29	0.47
1:D:108:SER:HB2	1:D:133:LYS:HD2	1.97	0.47
1:G:267:THR:HG1	1:G:271:ARG:NH2	2.13	0.47
1:G:266:ASP:O	1:G:270:ASN:HB2	2.13	0.47
1:E:121:ARG:HB2	1:F:121:ARG:HB2	1.97	0.47
1:F:109:THR:HA	1:F:196:VAL:HG21	1.95	0.47
1:A:244:LEU:HD12	1:B:244:LEU:HD13	1.96	0.47
1:E:142:PHE:O	1:E:143:ARG:NH1	2.42	0.47
1:H:108:SER:O	1:H:110:PRO:HD3	2.15	0.47
1:H:139:TRP:CD1	1:H:217:PRO:HD2	2.49	0.47
1:B:167:PRO:HG3	1:B:187:GLY:HA3	1.97	0.47
1:D:218:GLY:H	1:D:221:ASP:HB2	1.79	0.47
1:C:217:PRO:HG3	1:C:225:GLU:HB2	1.97	0.47
1:D:205:LEU:HD12	1:D:206:ALA:H	1.78	0.47
1:E:182:GLU:O	1:E:186:LEU:HG	2.14	0.47
1:C:234:GLU:OE1	1:C:234:GLU:N	2.45	0.46
1:A:121:ARG:HB3	1:B:120:GLU:C	2.35	0.46
1:D:232:THR:O	1:D:233:LEU:HB2	2.14	0.46
1:C:118:MSE:HE2	1:C:118:MSE:HB3	1.89	0.46
1:F:106:ARG:C	1:F:108:SER:H	2.17	0.46
1:F:130:LEU:HD13	1:F:140:VAL:HG22	1.98	0.46
1:C:120:GLU:O	1:C:121:ARG:HD2	2.16	0.46
1:G:118:MSE:SE	1:G:126:VAL:HG21	2.66	0.46
1:C:137:GLU:HG3	1:C:138:SER:H	1.81	0.46
1:C:108:SER:O	1:C:196:VAL:HG21	2.16	0.46
1:A:242:LYS:O	1:A:246:GLU:HG2	2.16	0.46
1:D:169:LYS:H	1:D:169:LYS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:TRP:HB2	1:F:217:PRO:HD2	1.97	0.46
1:G:170:ARG:C	1:G:172:PHE:H	2.19	0.46
1:E:110:PRO:HD2	1:E:196:VAL:HG21	1.98	0.46
1:F:110:PRO:HD2	1:F:196:VAL:HG11	1.97	0.46
1:F:120:GLU:O	1:F:122:ALA:N	2.49	0.46
1:B:246:GLU:O	1:B:249:LYS:HB3	2.16	0.45
1:A:169:LYS:HG3	1:A:171:TRP:N	2.25	0.45
1:D:188:LEU:O	1:D:191:PHE:HB3	2.16	0.45
1:D:120:GLU:O	1:D:120:GLU:HG3	2.15	0.45
1:E:278:GLU:H	1:E:278:GLU:HG3	1.53	0.45
1:F:198:HIS:HB3	1:F:201:ILE:HB	1.97	0.45
1:G:109:THR:HA	1:G:110:PRO:HD2	1.82	0.45
1:F:148:PHE:HZ	1:F:192:LEU:HD21	1.80	0.45
1:D:191:PHE:O	1:D:195:LEU:HG	2.17	0.45
1:F:110:PRO:HB3	1:F:131:VAL:HG22	1.98	0.45
1:D:261:LYS:O	1:D:265:ILE:HG12	2.16	0.45
1:E:170:ARG:NH1	1:E:184:ARG:HH12	2.14	0.45
1:E:217:PRO:HB2	1:E:221:ASP:HB2	1.98	0.45
1:A:272:ILE:O	1:A:276:SER:HB3	2.16	0.45
1:F:204:CYS:SG	1:F:207:VAL:HB	2.57	0.45
1:G:156:LYS:HA	1:G:156:LYS:HD2	1.74	0.45
1:G:144:ARG:H	1:G:144:ARG:HG2	1.54	0.45
1:A:170:ARG:H	1:A:170:ARG:HD3	1.82	0.45
1:B:150:ARG:NE	1:B:239:ARG:HH12	2.15	0.45
1:B:272:ILE:O	1:B:276:SER:OG	2.26	0.45
1:E:272:ILE:HD12	1:E:272:ILE:HA	1.68	0.45
1:F:195:LEU:O	1:F:201:ILE:HG21	2.15	0.45
1:G:262:GLN:HB3	1:H:261:LYS:HE3	1.99	0.45
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.83	0.45
1:C:135:PRO:C	1:C:137:GLU:H	2.19	0.45
1:A:223:LEU:O	1:A:226:SER:HB3	2.17	0.44
1:C:259:SER:O	1:C:262:GLN:HG3	2.17	0.44
1:E:256:LYS:HE2	1:E:260:GLU:OE2	2.17	0.44
1:G:139:TRP:CD2	1:G:217:PRO:HG2	2.52	0.44
1:H:198:HIS:ND1	1:H:199:LYS:O	2.51	0.44
1:A:132:LYS:HE3	1:A:135:PRO:HA	1.99	0.44
1:C:177:ASN:OD1	1:C:179:ASP:HB2	2.18	0.44
1:C:265:ILE:HG12	1:D:265:ILE:HG23	2.00	0.44
1:F:170:ARG:O	1:F:171:TRP:CD1	2.71	0.44
1:G:247:LYS:HG3	1:H:251:MSE:HE1	2.00	0.43
1:A:158:MSE:HE2	1:A:158:MSE:HB3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:LYS:O	1:F:132:LYS:HD3	2.17	0.43
1:H:242:LYS:O	1:H:246:GLU:HG3	2.18	0.43
1:D:113:LEU:HD11	1:D:130:LEU:HB2	1.99	0.43
1:D:139:TRP:CD1	1:D:217:PRO:HD2	2.54	0.43
1:E:199:LYS:O	1:E:201:ILE:N	2.52	0.43
1:G:166:LEU:HD22	1:G:169:LYS:HD2	2.01	0.43
1:C:231:GLU:OE2	1:C:239:ARG:NE	2.43	0.43
1:E:151:LEU:O	1:E:155:LEU:HG	2.19	0.43
1:F:174:ASP:HB3	1:F:177:ASN:HB2	2.00	0.43
1:G:129:ILE:HB	1:G:141:VAL:HG23	2.01	0.43
1:G:177:ASN:HB3	1:G:178:ALA:H	1.65	0.43
1:H:126:VAL:HG21	1:H:142:PHE:HB3	2.00	0.43
1:A:171:TRP:HA	1:A:171:TRP:CE3	2.54	0.43
1:C:226:SER:OG	1:C:227:ARG:N	2.51	0.43
1:A:208:ARG:HG2	1:A:213:LEU:HB2	1.99	0.43
1:G:180:PHE:CZ	1:G:184:ARG:NE	2.87	0.43
1:D:113:LEU:HD23	1:D:113:LEU:HA	1.83	0.43
1:H:166:LEU:HD12	1:H:166:LEU:HA	1.85	0.43
1:F:174:ASP:C	1:F:176:TYR:H	2.21	0.42
1:H:162:PHE:HE1	1:H:201:ILE:HD11	1.79	0.42
1:A:179:ASP:HB3	1:A:180:PHE:H	1.70	0.42
1:F:113:LEU:HB2	1:F:128:LYS:HB2	2.02	0.42
1:B:139:TRP:CG	1:B:216:PRO:HB2	2.55	0.42
1:B:199:LYS:O	1:B:200:ASP:HB2	2.20	0.42
1:B:201:ILE:O	1:B:207:VAL:HG11	2.20	0.42
1:D:191:PHE:CE2	1:D:195:LEU:HD11	2.54	0.42
1:G:139:TRP:CG	1:G:217:PRO:HG2	2.54	0.42
1:H:139:TRP:HZ2	1:H:213:LEU:HD23	1.85	0.42
1:B:170:ARG:NE	1:B:173:LYS:HB3	2.34	0.42
1:C:105:ASP:HB3	1:C:203:ASN:ND2	2.32	0.42
1:E:108:SER:HB2	1:E:132:LYS:O	2.20	0.42
1:E:269:GLU:O	1:E:272:ILE:HG22	2.20	0.42
1:F:148:PHE:CE1	1:F:210:PHE:HZ	2.37	0.42
1:F:218:GLY:N	1:F:221:ASP:HB3	2.27	0.42
1:B:223:LEU:O	1:B:226:SER:HB3	2.20	0.42
1:D:118:MSE:SE	1:D:126:VAL:HG11	2.70	0.42
1:G:248:GLN:HG3	1:G:249:LYS:N	2.35	0.42
1:C:106:ARG:HH11	1:C:199:LYS:HE3	1.84	0.42
1:E:198:HIS:O	1:E:198:HIS:CG	2.73	0.42
1:F:172:PHE:HB2	1:F:173:LYS:H	1.69	0.42
1:B:257:LEU:O	1:B:261:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LYS:HG2	1:D:142:PHE:CE1	2.55	0.42
1:D:108:SER:O	1:D:196:VAL:HG11	2.20	0.41
1:C:258:LEU:HD13	1:D:258:LEU:HB2	2.02	0.41
1:G:152:ASN:HD22	1:G:165:ALA:HA	1.85	0.41
1:C:119:GLU:O	1:C:121:ARG:N	2.52	0.41
1:H:115:TYR:CD1	1:H:115:TYR:C	2.93	0.41
1:D:198:HIS:HB2	1:D:201:ILE:HB	2.02	0.41
1:A:121:ARG:HG3	1:B:120:GLU:HB2	2.02	0.41
1:C:184:ARG:HA	1:C:184:ARG:HD3	1.87	0.41
1:F:120:GLU:C	1:F:122:ALA:H	2.24	0.41
1:F:167:PRO:HA	1:F:168:PRO:HD3	1.85	0.41
1:B:106:ARG:HD3	1:B:106:ARG:HA	1.78	0.41
1:A:145:TYR:CG	1:A:184:ARG:NH1	2.89	0.41
1:E:199:LYS:O	1:E:202:ALA:N	2.36	0.41
1:F:105:ASP:OD1	1:F:105:ASP:N	2.53	0.41
1:H:142:PHE:HB2	1:H:226:SER:HB2	2.01	0.41
1:H:201:ILE:HG21	1:H:201:ILE:HD13	1.82	0.41
1:C:112:ILE:HG12	1:C:129:ILE:HG12	2.01	0.41
1:E:175:ASN:HB3	1:E:180:PHE:CD2	2.55	0.41
1:F:115:TYR:HB3	1:F:127:TYR:CD1	2.56	0.41
1:H:120:GLU:C	1:H:122:ALA:N	2.74	0.41
1:F:205:LEU:HD23	1:F:205:LEU:HA	1.75	0.41
1:A:208:ARG:HG3	1:A:213:LEU:HD12	2.02	0.40
1:G:129:ILE:HG21	1:G:211:LEU:CD2	2.47	0.40
1:G:145:TYR:O	1:G:148:PHE:HB2	2.20	0.40
1:C:106:ARG:HB3	1:C:106:ARG:CZ	2.51	0.40
1:D:239:ARG:O	1:D:243:GLU:HG3	2.20	0.40
1:F:133:LYS:HB3	1:F:139:TRP:CH2	2.57	0.40
1:F:276:SER:OG	1:F:277:LEU:HD23	2.22	0.40
1:B:150:ARG:HD3	1:B:239:ARG:NH1	2.33	0.40
1:F:148:PHE:CD2	1:F:188:LEU:HD22	2.41	0.40
1:F:167:PRO:CG	1:F:184:ARG:HA	2.46	0.40
1:F:265:ILE:HG13	1:F:266:ASP:N	2.34	0.40
1:H:151:LEU:O	1:H:155:LEU:HG	2.21	0.40
1:B:112:ILE:H	1:B:189:GLN:HE22	1.69	0.40
1:G:242:LYS:HD2	1:G:242:LYS:HA	1.70	0.40
1:H:181:LEU:HD23	1:H:181:LEU:HA	1.80	0.40
1:D:231:GLU:CD	1:D:239:ARG:HH21	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	173/179 (97%)	161 (93%)	10 (6%)	2 (1%)	13	44
1	B	171/179 (96%)	154 (90%)	15 (9%)	2 (1%)	13	44
1	C	174/179 (97%)	158 (91%)	12 (7%)	4 (2%)	6	31
1	D	170/179 (95%)	153 (90%)	16 (9%)	1 (1%)	25	59
1	E	174/179 (97%)	161 (92%)	12 (7%)	1 (1%)	25	59
1	F	167/179 (93%)	147 (88%)	11 (7%)	9 (5%)	2	13
1	G	157/179 (88%)	133 (85%)	24 (15%)	0	100	100
1	H	171/179 (96%)	159 (93%)	10 (6%)	2 (1%)	13	44
All	All	1357/1432 (95%)	1226 (90%)	110 (8%)	21 (2%)	10	39

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	ARG
1	F	121	ARG
1	H	121	ARG
1	A	222	SER
1	C	200	ASP
1	E	200	ASP
1	F	170	ARG
1	A	180	PHE
1	D	121	ARG
1	F	224	GLU
1	C	120	GLU
1	C	136	GLU
1	F	206	ALA
1	F	173	LYS
1	F	205	LEU
1	F	108	SER
1	F	168	PRO

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Mol	Chain	Res	Type
1	F	174	ASP
1	H	178	ALA
1	B	219	PRO
1	C	161	GLY

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	163/164 (99%)	153 (94%)	10 (6%)	18	50
1	B	161/164 (98%)	150 (93%)	11 (7%)	16	46
1	C	164/164 (100%)	148 (90%)	16 (10%)	8	30
1	D	160/164 (98%)	142 (89%)	18 (11%)	6	23
1	E	164/164 (100%)	148 (90%)	16 (10%)	8	30
1	F	159/164 (97%)	140 (88%)	19 (12%)	5	20
1	G	154/164 (94%)	135 (88%)	19 (12%)	4	19
1	H	161/164 (98%)	148 (92%)	13 (8%)	11	38
All	All	1286/1312 (98%)	1164 (90%)	122 (10%)	8	31

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
1	A	130	LEU
1	A	131	VAL
1	A	170	ARG
1	A	223	LEU
1	A	241	GLN
1	A	244	LEU
1	A	266	ASP
1	A	270	ASN
1	A	275	LEU
1	B	144	ARG

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Mol	Chain	Res	Type
1	B	162	PHE
1	B	179	ASP
1	B	205	LEU
1	B	214	ASP
1	B	215	ASP
1	B	220	PHE
1	B	223	LEU
1	B	241	GLN
1	B	273	ARG
1	B	274	THR
1	C	105	ASP
1	C	106	ARG
1	C	170	ARG
1	C	184	ARG
1	C	205	LEU
1	C	223	LEU
1	C	227	ARG
1	C	244	LEU
1	C	255	LYS
1	C	262	GLN
1	C	263	LEU
1	C	268	LEU
1	C	270	ASN
1	C	271	ARG
1	C	277	LEU
1	C	278	GLU
1	D	106	ARG
1	D	111	THR
1	D	121	ARG
1	D	133	LYS
1	D	140	VAL
1	D	156	LYS
1	D	171	TRP
1	D	200	ASP
1	D	205	LEU
1	D	213	LEU
1	D	215	ASP
1	D	241	GLN
1	D	251	MSE
1	D	252	GLU
1	D	258	LEU
1	D	270	ASN

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Mol	Chain	Res	Type
1	D	273	ARG
1	D	277	LEU
1	E	128	LYS
1	E	136	GLU
1	E	150	ARG
1	E	154	LYS
1	E	169	LYS
1	E	170	ARG
1	E	193	GLN
1	E	199	LYS
1	E	204	CYS
1	E	250	GLU
1	E	251	MSE
1	E	257	LEU
1	E	263	LEU
1	E	272	ILE
1	E	277	LEU
1	E	278	GLU
1	F	115	TYR
1	F	116	GLU
1	F	121	ARG
1	F	144	ARG
1	F	150	ARG
1	F	158	MSE
1	F	162	PHE
1	F	169	LYS
1	F	170	ARG
1	F	181	LEU
1	F	182	GLU
1	F	201	ILE
1	F	220	PHE
1	F	234	GLU
1	F	241	GLN
1	F	242	LYS
1	F	265	ILE
1	F	273	ARG
1	F	277	LEU
1	G	117	VAL
1	G	136	GLU
1	G	137	GLU
1	G	139	TRP
1	G	142	PHE

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Mol	Chain	Res	Type
1	G	144	ARG
1	G	145	TYR
1	G	155	LEU
1	G	166	LEU
1	G	191	PHE
1	G	203	ASN
1	G	212	CYS
1	G	225	GLU
1	G	247	LYS
1	G	248	GLN
1	G	260	GLU
1	G	266	ASP
1	G	268	LEU
1	G	277	LEU
1	H	106	ARG
1	H	109	THR
1	H	115	TYR
1	H	120	GLU
1	H	164	LEU
1	H	170	ARG
1	H	184	ARG
1	H	200	ASP
1	H	244	LEU
1	H	251	MSE
1	H	256	LYS
1	H	258	LEU
1	H	264	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	203	ASN
1	E	193	GLN
1	F	189	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

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, 95th 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	172/179 (96%)	0.12	0 100 100	24, 53, 84, 100	0
1	B	170/179 (94%)	0.41	15 (8%) 10 11	48, 94, 140, 167	0
1	C	173/179 (96%)	0.23	7 (4%) 38 40	37, 73, 203, 246	0
1	D	169/179 (94%)	0.18	4 (2%) 59 61	31, 64, 169, 195	0
1	E	173/179 (96%)	0.10	1 (0%) 89 92	23, 52, 104, 131	0
1	F	168/179 (93%)	0.38	10 (5%) 21 24	71, 107, 163, 181	0
1	G	162/179 (90%)	0.60	16 (9%) 7 8	75, 139, 185, 208	0
1	H	170/179 (94%)	0.31	8 (4%) 31 34	14, 39, 183, 207	0
All	All	1357/1432 (94%)	0.29	61 (4%) 33 36	14, 80, 169, 246	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	278	GLU	5.8
1	H	276	SER	5.4
1	F	219	PRO	4.9
1	G	140	VAL	4.9
1	G	141	VAL	4.3
1	G	192	LEU	4.1
1	B	132	LYS	3.7
1	H	272	ILE	3.7
1	G	276	SER	3.7
1	H	264	HIS	3.5
1	B	110	PRO	3.5
1	C	122	ALA	3.5
1	G	263	LEU	3.4
1	F	141	VAL	3.3
1	B	212	CYS	3.2
1	G	261	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	129	ILE	3.0
1	G	258	LEU	3.0
1	F	222	SER	2.9
1	B	112	ILE	2.8
1	F	210	PHE	2.8
1	H	269	GLU	2.7
1	H	273	ARG	2.7
1	B	113	LEU	2.6
1	B	140	VAL	2.6
1	H	203	ASN	2.6
1	F	212	CYS	2.6
1	C	277	LEU	2.6
1	C	276	SER	2.5
1	B	211	LEU	2.5
1	B	138	SER	2.5
1	G	177	ASN	2.5
1	C	268	LEU	2.5
1	B	107	PRO	2.5
1	E	175	ASN	2.5
1	B	196	VAL	2.5
1	F	129	ILE	2.4
1	F	131	VAL	2.4
1	G	273	ARG	2.4
1	B	121	ARG	2.4
1	D	274	THR	2.4
1	B	129	ILE	2.4
1	G	264	HIS	2.3
1	G	160	PRO	2.3
1	D	264	HIS	2.3
1	G	212	CYS	2.2
1	D	272	ILE	2.2
1	H	258	LEU	2.2
1	F	130	LEU	2.2
1	B	127	TYR	2.2
1	F	231	GLU	2.2
1	G	271	ARG	2.1
1	D	263	LEU	2.1
1	G	230	CYS	2.1
1	G	200	ASP	2.1
1	B	105	ASP	2.1
1	B	210	PHE	2.0
1	F	230	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	268	LEU	2.0
1	C	128	LYS	2.0
1	C	121	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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.