



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:47 PM GMT

PDB ID : 4DGW
Title : Crystal Structure of the SF3a splicing factor complex of U2 snRNP
Authors : Lin, P.C.
Deposited on : 2012-01-26
Resolution : 3.11 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

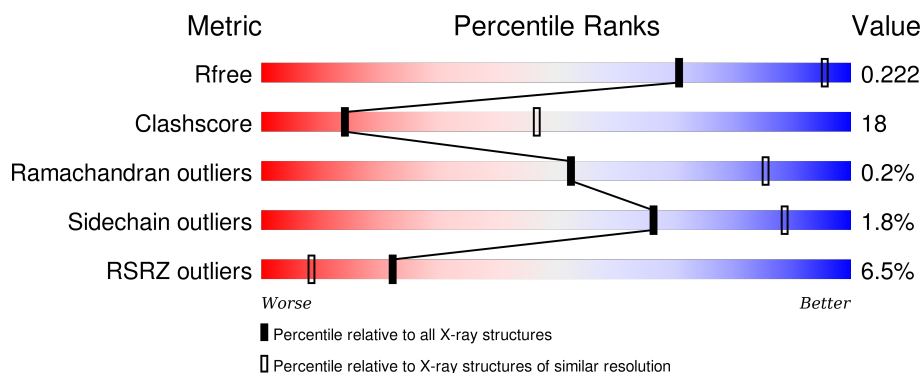
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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.

Mol	Chain	Length	Quality of chain
1	A	402	<div> <div>3%</div> <div>58%</div> <div>33%</div> <div>9%</div> </div>
2	B	152	<div> <div>4%</div> <div>52%</div> <div>30%</div> <div>16%</div> </div>
3	C	231	<div> <div>8%</div> <div>42%</div> <div>19%</div> <div>39%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5195 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 Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	365	3095	1969	531	584	4	7	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	EXPRESSION TAG	UNP P19736
A	-11	SER	-	EXPRESSION TAG	UNP P19736
A	-10	PRO	-	EXPRESSION TAG	UNP P19736
A	-9	GLY	-	EXPRESSION TAG	UNP P19736
A	-8	ILE	-	EXPRESSION TAG	UNP P19736
A	-7	SER	-	EXPRESSION TAG	UNP P19736
A	-6	GLY	-	EXPRESSION TAG	UNP P19736
A	-5	GLY	-	EXPRESSION TAG	UNP P19736
A	-4	GLY	-	EXPRESSION TAG	UNP P19736
A	-3	GLY	-	EXPRESSION TAG	UNP P19736
A	-2	ILE	-	EXPRESSION TAG	UNP P19736
A	-1	LEU	-	EXPRESSION TAG	UNP P19736
A	0	GLU	-	EXPRESSION TAG	UNP P19736

- Molecule 2 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	127	1084	689	193	196	2	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	86	MSE	-	EXPRESSION TAG	UNP P32524

- Molecule 3 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	141	Total	C	N	O	S	Se	0	0	0
			1008	632	168	205	1	2			

There are 15 discrepancies between the modelled and reference sequences:

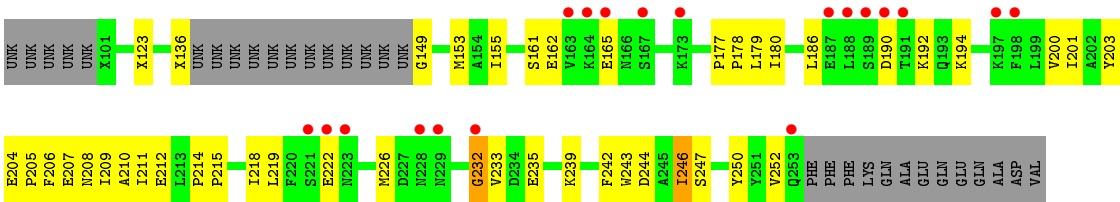
Chain	Residue	Modelled	Actual	Comment	Reference
C	36	UNK	-	SEE REAMRK 999	UNP Q07350
C	37	UNK	-	SEE REAMRK 999	UNP Q07350
C	38	UNK	-	SEE REAMRK 999	UNP Q07350
C	39	UNK	-	SEE REAMRK 999	UNP Q07350
C	40	UNK	-	SEE REAMRK 999	UNP Q07350
C	41	UNK	-	SEE REAMRK 999	UNP Q07350
C	42	UNK	-	SEE REAMRK 999	UNP Q07350
C	43	UNK	-	SEE REAMRK 999	UNP Q07350
C	44	UNK	-	SEE REAMRK 999	UNP Q07350
C	45	UNK	-	SEE REAMRK 999	UNP Q07350
C	46	UNK	-	SEE REAMRK 999	UNP Q07350
C	47	UNK	-	SEE REAMRK 999	UNP Q07350
C	48	UNK	-	SEE REAMRK 999	UNP Q07350
C	49	UNK	-	SEE REAMRK 999	UNP Q07350
C	153	MSE	LEU	ENGINEERED MUTATION	UNP Q07350

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	1	Total	O	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.78 Å 127.26 Å 169.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 3.11 29.86 – 3.11	Depositor EDS
% Data completeness (in resolution range)	96.6 (29.86-3.11) 96.4 (29.86-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.11 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.228 , 0.278 0.235 , 0.222	Depositor DCC
R_{free} test set	976 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	94.5	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19170 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5195	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.26	0/3148	0.40	0/4207
2	B	0.23	0/1101	0.37	0/1463
3	C	0.22	0/840	0.40	0/1133
All	All	0.25	0/5089	0.39	0/6803

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3095	0	3066	113	0
2	B	1084	0	1081	51	0
3	C	1008	0	854	43	0
4	A	1	0	0	0	0
5	A	6	0	0	0	0
5	B	1	0	0	0	0
All	All	5195	0	5001	185	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 18.

All (185) 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)
3:C:235:GLU:O	3:C:239:LYS:HB2	1.69	0.92
1:A:63:LYS:HB2	1:A:376:GLN:HG3	1.49	0.92
1:A:331:GLU:O	1:A:335:THR:HG23	1.79	0.81
1:A:150:PRO:HB3	1:A:154:THR:HB	1.64	0.79
1:A:150:PRO:HG3	1:A:154:THR:H	1.46	0.79
3:C:180:ILE:HG22	3:C:201:ILE:HG12	1.67	0.76
2:B:103:TYR:HD1	2:B:110:VAL:HG21	1.53	0.74
2:B:92:ASP:O	2:B:96:ILE:HG12	1.89	0.73
1:A:93:PHE:CZ	2:B:148:PHE:HE1	2.06	0.73
3:C:123:UNK:HA	3:C:207:GLU:HB2	1.72	0.72
2:B:158:ARG:HB2	2:B:158:ARG:HH11	1.53	0.72
1:A:150:PRO:HG3	1:A:155:ASN:H	1.55	0.71
1:A:377:VAL:O	1:A:378:ASP:HB2	1.91	0.71
3:C:246:ILE:H	3:C:246:ILE:HD13	1.54	0.71
1:A:33:TYR:O	1:A:36:ILE:HG22	1.91	0.71
2:B:192:PHE:HB2	3:C:179:LEU:HD13	1.72	0.71
1:A:93:PHE:HZ	2:B:148:PHE:HE1	1.39	0.71
3:C:186:LEU:HA	3:C:194:LYS:HD2	1.71	0.70
3:C:203:TYR:HD2	3:C:205:PRO:HD2	1.57	0.69
3:C:153:MSE:H	3:C:219:LEU:HD23	1.58	0.67
2:B:132:HIS:O	2:B:135:PHE:HB3	1.94	0.67
1:A:116:LEU:HD13	2:B:102:TYR:CD2	2.30	0.67
1:A:148:SER:HB2	1:A:159:ASP:H	1.58	0.67
2:B:97:LYS:O	2:B:101:ARG:HG3	1.93	0.67
3:C:212:GLU:HG2	3:C:214:PRO:HD3	1.76	0.67
3:C:136:UNK:HA	3:C:149:GLY:HA2	1.77	0.67
2:B:221:LEU:O	2:B:225:ARG:HG3	1.95	0.66
1:A:180:MSE:H	1:A:335:THR:HG21	1.62	0.65
1:A:81:ILE:HD11	1:A:160:ARG:HG3	1.79	0.65
3:C:178:PRO:HD3	3:C:203:TYR:HE1	1.61	0.65
1:A:139:ASP:O	1:A:143:LEU:HB2	1.96	0.65
1:A:132:LEU:HD23	1:A:132:LEU:H	1.61	0.64
3:C:218:ILE:O	3:C:219:LEU:HG	2.00	0.62
1:A:63:LYS:HE3	1:A:378:ASP:HB2	1.82	0.61
3:C:178:PRO:HD3	3:C:203:TYR:CE1	2.35	0.61
1:A:26:GLN:HB2	2:B:168:THR:HG23	1.83	0.60
1:A:179:TYR:HA	1:A:335:THR:HG22	1.83	0.60
2:B:225:ARG:HG2	3:C:242:PHE:HD1	1.66	0.60
1:A:243:PHE:HA	1:A:246:LYS:HE2	1.83	0.60
1:A:148:SER:HB2	1:A:159:ASP:N	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HG3	1:A:59:ILE:HG13	1.84	0.59
1:A:31:LEU:HD11	1:A:75:GLN:OE1	2.02	0.58
2:B:185:VAL:HG13	3:C:232:GLY:HA2	1.83	0.58
1:A:170:PHE:CZ	1:A:246:LYS:HG2	2.39	0.58
3:C:214:PRO:N	3:C:215:PRO:HD2	2.19	0.58
2:B:225:ARG:HG2	3:C:242:PHE:CD1	2.38	0.58
2:B:134:THR:O	2:B:137:ASP:HB2	2.04	0.58
1:A:14:MSE:HE3	1:A:86:TYR:CZ	2.39	0.58
1:A:377:VAL:HG12	1:A:378:ASP:N	2.19	0.58
2:B:192:PHE:CD2	3:C:233:VAL:HG11	2.39	0.58
2:B:140:ALA:HA	2:B:143:LYS:HD2	1.85	0.57
1:A:377:VAL:HG12	1:A:378:ASP:H	1.69	0.56
1:A:199:SER:H	1:A:202:GLN:HE21	1.53	0.56
1:A:150:PRO:CB	1:A:154:THR:HB	2.36	0.56
1:A:148:SER:HB2	1:A:158:SER:HA	1.87	0.55
1:A:148:SER:CB	1:A:159:ASP:H	2.20	0.55
1:A:21:ILE:HD11	2:B:164:CYS:SG	2.47	0.55
1:A:93:PHE:HZ	2:B:148:PHE:CE1	2.24	0.54
1:A:319:TYR:O	1:A:322:HIS:HB3	2.08	0.54
1:A:147:SER:HA	1:A:155:ASN:O	2.08	0.54
1:A:251:LEU:HD12	1:A:251:LEU:O	2.08	0.53
1:A:62:PHE:HB3	1:A:375:GLU:HB2	1.89	0.53
2:B:129:HIS:ND1	2:B:130:PRO:HD2	2.23	0.53
2:B:205:LYS:HB3	3:C:212:GLU:HB3	1.90	0.53
3:C:204:GLU:HB3	3:C:205:PRO:HD3	1.91	0.53
2:B:202:GLN:HB3	3:C:210:ALA:HB3	1.91	0.53
2:B:103:TYR:CD1	2:B:110:VAL:HG21	2.40	0.53
3:C:123:UNK:C	3:C:207:GLU:HB2	2.39	0.53
1:A:90:GLN:HG3	2:B:153:ILE:HG13	1.90	0.52
1:A:220:PRO:HB2	1:A:222:MSE:O	2.10	0.52
3:C:123:UNK:CA	3:C:207:GLU:HB2	2.40	0.51
1:A:81:ILE:HD13	1:A:161:ALA:HB2	1.92	0.51
2:B:195:ILE:HD11	2:B:197:TRP:CZ2	2.45	0.51
1:A:185:PHE:CE2	1:A:236:LEU:HA	2.46	0.51
1:A:302:LYS:O	1:A:306:LYS:HG2	2.11	0.51
1:A:237:SER:HA	1:A:321:LEU:HD13	1.94	0.50
1:A:171:THR:HG21	1:A:181:GLU:OE2	2.11	0.50
1:A:292:SER:O	1:A:296:GLU:HG2	2.10	0.50
1:A:75:GLN:HE21	1:A:156:ILE:HG21	1.76	0.50
1:A:342:LYS:HA	1:A:345:PHE:CD2	2.47	0.50
3:C:153:MSE:HE1	3:C:211:ILE:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:OE1	1:A:63:LYS:HE2	2.11	0.50
1:A:14:MSE:HE3	1:A:86:TYR:OH	2.11	0.50
1:A:115:LYS:HA	1:A:118:GLN:HB3	1.93	0.50
1:A:91:GLN:HG2	1:A:95:LYS:HE2	1.94	0.50
1:A:206:ILE:HG23	1:A:221:PRO:HG3	1.94	0.49
1:A:11:LEU:HD11	2:B:148:PHE:HZ	1.77	0.49
2:B:139:VAL:O	2:B:143:LYS:HG3	2.12	0.49
3:C:190:ASP:HB2	3:C:192:LYS:HE3	1.94	0.49
1:A:117:GLN:HB3	2:B:113:MSE:HE3	1.94	0.48
2:B:191:GLN:O	2:B:195:ILE:HG23	2.12	0.48
1:A:267:SER:O	1:A:272:SER:HB2	2.13	0.48
2:B:141:GLN:O	2:B:144:ARG:HB2	2.13	0.48
1:A:377:VAL:O	1:A:378:ASP:CB	2.60	0.48
1:A:26:GLN:CB	2:B:168:THR:HG23	2.42	0.48
1:A:192:VAL:HG12	1:A:222:MSE:HE1	1.95	0.48
1:A:208:GLU:HG3	1:A:332:PHE:CE1	2.49	0.48
1:A:62:PHE:HA	1:A:376:GLN:O	2.14	0.48
1:A:31:LEU:HD23	1:A:72:ILE:HG23	1.96	0.48
1:A:195:ARG:HD3	1:A:197:ASP:OD2	2.14	0.48
3:C:155:ILE:HD12	3:C:155:ILE:N	2.29	0.47
2:B:127:SER:HA	2:B:132:HIS:CG	2.50	0.47
1:A:178:GLU:HA	1:A:334:ARG:HH11	1.78	0.47
2:B:99:THR:HG21	2:B:122:LEU:HD22	1.97	0.47
1:A:219:THR:N	1:A:220:PRO:HD3	2.30	0.47
3:C:155:ILE:HB	3:C:252:VAL:CG2	2.44	0.47
1:A:210:PHE:CE1	1:A:216:TYR:HB2	2.49	0.47
1:A:193:ILE:HG22	1:A:222:MSE:HE2	1.96	0.47
3:C:244:ASP:OD2	3:C:247:SER:HB3	2.14	0.47
1:A:169:ILE:O	1:A:246:LYS:HD2	2.15	0.46
2:B:108:SER:O	2:B:112:GLN:HG3	2.16	0.46
1:A:264:PHE:CE1	1:A:268:TYR:CD2	3.04	0.46
2:B:158:ARG:HB2	2:B:158:ARG:NH1	2.25	0.46
1:A:60:TYR:CE2	1:A:61:LYS:HG2	2.51	0.46
1:A:7:ARG:HD2	1:A:96:ILE:HG22	1.97	0.46
3:C:165:GLU:HG2	3:C:165:GLU:O	2.16	0.46
2:B:139:VAL:HG23	2:B:140:ALA:H	1.80	0.46
1:A:188:LEU:O	1:A:192:VAL:HG23	2.16	0.45
1:A:4:LEU:HD21	2:B:146:TYR:OH	2.16	0.45
1:A:12:GLU:O	1:A:16:ILE:HG13	2.15	0.45
2:B:106:ASP:O	2:B:107:LYS:HB2	2.16	0.45
1:A:150:PRO:CG	1:A:154:THR:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:LYS:CB	3:C:212:GLU:HB3	2.46	0.45
1:A:156:ILE:HG12	1:A:366:TYR:HB2	1.97	0.45
1:A:180:MSE:H	1:A:335:THR:CG2	2.28	0.45
2:B:99:THR:O	2:B:103:TYR:HB2	2.17	0.45
1:A:175:GLN:HB2	1:A:178:GLU:HB3	1.99	0.45
2:B:139:VAL:HG23	2:B:140:ALA:N	2.33	0.44
1:A:169:ILE:HG22	1:A:246:LYS:CD	2.47	0.44
1:A:34:HIS:CD2	1:A:76:GLN:HE22	2.35	0.44
3:C:200:VAL:HA	3:C:209:ILE:O	2.18	0.44
1:A:117:GLN:HB3	2:B:113:MSE:CE	2.47	0.44
2:B:113:MSE:SE	2:B:117:ASP:HB2	2.67	0.44
2:B:181:HIS:O	2:B:185:VAL:HG23	2.18	0.44
3:C:177:PRO:HB3	3:C:243:TRP:CD1	2.53	0.44
3:C:153:MSE:HE1	3:C:211:ILE:HD13	2.00	0.44
1:A:212:ASP:HB3	1:A:215:LYS:HB2	2.00	0.44
1:A:21:ILE:O	1:A:25:ILE:HG13	2.18	0.44
1:A:178:GLU:O	1:A:334:ARG:HD2	2.17	0.44
1:A:355:ASP:O	1:A:359:GLN:HG2	2.17	0.44
1:A:172:ARG:HG3	1:A:361:TYR:HB2	1.99	0.44
1:A:38:GLU:O	1:A:41:LYS:HG2	2.18	0.43
1:A:264:PHE:CE1	1:A:268:TYR:HD2	2.37	0.43
1:A:219:THR:O	1:A:219:THR:HG22	2.17	0.43
1:A:203:PHE:O	1:A:206:ILE:HB	2.18	0.43
1:A:267:SER:C	1:A:272:SER:HB2	2.39	0.43
3:C:155:ILE:HD13	3:C:252:VAL:HG23	2.00	0.43
3:C:222:GLU:HG3	3:C:222:GLU:O	2.19	0.43
3:C:178:PRO:HG2	3:C:250:TYR:CD1	2.52	0.43
2:B:195:ILE:HD11	2:B:197:TRP:CH2	2.54	0.43
2:B:119:GLU:C	2:B:121:ARG:H	2.21	0.42
3:C:178:PRO:O	3:C:179:LEU:HD23	2.19	0.42
1:A:202:GLN:O	1:A:206:ILE:HG13	2.20	0.42
1:A:217:LEU:HA	1:A:217:LEU:HD12	1.82	0.42
3:C:214:PRO:N	3:C:215:PRO:CD	2.83	0.42
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.91	0.42
1:A:226:ASN:O	1:A:230:MSE:HG3	2.20	0.42
3:C:205:PRO:HG2	3:C:206:PHE:CD1	2.55	0.42
2:B:199:LYS:O	3:C:208:ASN:HB2	2.20	0.42
1:A:58:LYS:HB3	1:A:63:LYS:HA	2.02	0.42
1:A:359:GLN:OE1	1:A:359:GLN:HA	2.20	0.42
1:A:88:GLU:O	1:A:92:THR:HG23	2.20	0.42
3:C:219:LEU:HD12	3:C:219:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ILE:CD1	1:A:161:ALA:HB2	2.50	0.41
1:A:230:MSE:HA	1:A:314:PHE:CE1	2.55	0.41
3:C:161:SER:C	3:C:162:GLU:HG3	2.39	0.41
1:A:48:LEU:HD12	1:A:48:LEU:O	2.20	0.41
1:A:11:LEU:HD11	2:B:148:PHE:CZ	2.55	0.41
1:A:319:TYR:CZ	1:A:323:ARG:HD2	2.54	0.41
1:A:69:ARG:O	1:A:73:ILE:HG12	2.20	0.41
1:A:53:LEU:HD23	1:A:58:LYS:HE3	2.03	0.41
1:A:171:THR:HG22	1:A:174:GLU:CD	2.40	0.41
1:A:40:SER:HA	1:A:46:THR:OG1	2.20	0.41
1:A:149:ASP:N	1:A:150:PRO:HD2	2.36	0.41
2:B:135:PHE:O	2:B:139:VAL:HG22	2.21	0.41
2:B:140:ALA:O	2:B:143:LYS:HB2	2.21	0.41
3:C:178:PRO:HB3	3:C:203:TYR:HD1	1.85	0.41
1:A:116:LEU:HD11	1:A:120:GLU:OE2	2.20	0.41
2:B:226:LEU:O	2:B:227:ARG:HD3	2.20	0.41
1:A:377:VAL:CG1	1:A:378:ASP:H	2.33	0.41
1:A:192:VAL:HG13	1:A:228:ARG:HB3	2.02	0.40
1:A:150:PRO:HD3	1:A:155:ASN:HB3	2.04	0.40
1:A:181:GLU:HG3	1:A:181:GLU:O	2.22	0.40
1:A:36:ILE:HA	1:A:36:ILE:HD12	1.86	0.40
1:A:338:PHE:CZ	1:A:357:LEU:HD11	2.57	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	361/402 (90%)	330 (91%)	31 (9%)	0	100	100
2	B	123/152 (81%)	112 (91%)	11 (9%)	0	100	100
3	C	103/231 (45%)	83 (81%)	19 (18%)	1 (1%)	19	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	587/785 (75%)	525 (89%)	61 (10%)	1 (0%)	52 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	232	GLY

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	342/364 (94%)	337 (98%)	5 (2%)	72 90
2	B	118/135 (87%)	115 (98%)	3 (2%)	55 84
3	C	95/104 (91%)	93 (98%)	2 (2%)	61 86
All	All	555/603 (92%)	545 (98%)	10 (2%)	66 89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	35	TYR
1	A	81	ILE
1	A	298	HIS
1	A	317	SER
2	B	113	MSE
2	B	129	HIS
2	B	158	ARG
3	C	226	MSE
3	C	246	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	91	GLN
1	A	167	ASN
1	A	202	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	358/402 (89%)	-0.04	13 (3%) 46 23	66, 103, 211, 270	0
2	B	123/152 (80%)	0.15	6 (4%) 33 14	85, 160, 215, 223	0
3	C	103/231 (44%)	0.88	19 (18%) 2 1	115, 176, 242, 260	0
All	All	584/785 (74%)	0.16	38 (6%) 22 8	66, 124, 222, 270	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	PHE	5.8
1	A	128	GLU	4.9
3	C	189	SER	4.9
3	C	190	ASP	4.3
1	A	129	ASN	4.3
3	C	165	GLU	4.1
3	C	228	ASN	4.1
3	C	187	GLU	4.0
1	A	134	ILE	4.0
3	C	232	GLY	3.8
2	B	202	GLN	3.7
3	C	164	LYS	3.7
1	A	135	ASN	3.7
3	C	188	LEU	3.7
1	A	290	LYS	3.5
2	B	148	PHE	3.0
3	C	222	GLU	3.0
3	C	221	SER	3.0
2	B	91	ARG	3.0
3	C	198	PHE	2.9
3	C	253	GLN	2.8
1	A	141	TYR	2.8
1	A	131	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	229	ASN	2.8
3	C	191	THR	2.7
1	A	373	GLY	2.6
2	B	227	ARG	2.6
1	A	378	ASP	2.6
3	C	167	SER	2.5
3	C	163	VAL	2.4
3	C	173	LYS	2.4
2	B	106	ASP	2.3
1	A	133	ASP	2.3
3	C	197	LYS	2.2
2	B	130	PRO	2.2
3	C	223	ASN	2.2
1	A	376	GLN	2.1
1	A	377	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	A	401	1/1	0.99	0.22	-0.00	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.