



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 PM GMT

PDB ID : 4JGH
Title : Structure of the SOCS2-Elongin BC complex bound to an N-terminal fragment of Cullin5
Authors : Kim, Y.K.; Kwak, M.J.; Ku, B.; Suh, H.Y.; Joo, K.; Lee, J.; Jung, J.U.; Oh, B.H.
Deposited on : 2013-03-01
Resolution : 3.00 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

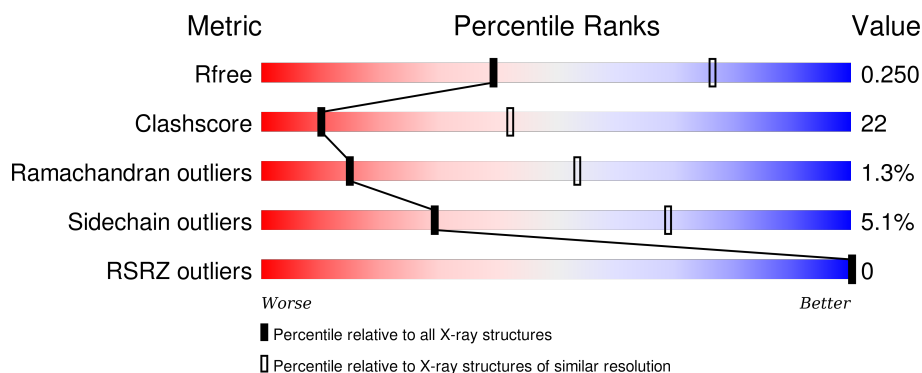
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	173	<div> <div>53%</div> <div>37%</div> <div>6%</div> </div>
2	B	118	<div> <div>52%</div> <div>36%</div> <div>12%</div> </div>
3	C	96	<div> <div>69%</div> <div>27%</div> <div></div> </div>
4	D	378	<div> <div>53%</div> <div>41%</div> <div></div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5902 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 Suppressor of cytokine signaling 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1310	842	220	242	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	HIS	-	EXPRESSION TAG	UNP O14508
A	27	MET	-	EXPRESSION TAG	UNP O14508
A	28	ASP	-	EXPRESSION TAG	UNP O14508
A	29	PRO	-	EXPRESSION TAG	UNP O14508
A	30	GLU	-	EXPRESSION TAG	UNP O14508
A	31	PHE	-	EXPRESSION TAG	UNP O14508

- Molecule 2 is a protein called Transcription elongation factor B polypeptide 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			828	524	141	159	4			

- Molecule 3 is a protein called Transcription elongation factor B polypeptide 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			762	489	122	145	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	PRO	ALA	SEE REMARK 999	UNP P83940

- Molecule 4 is a protein called Cullin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	368	Total	C	N	O	S	0	0	0
			3002	1907	509	568	18			

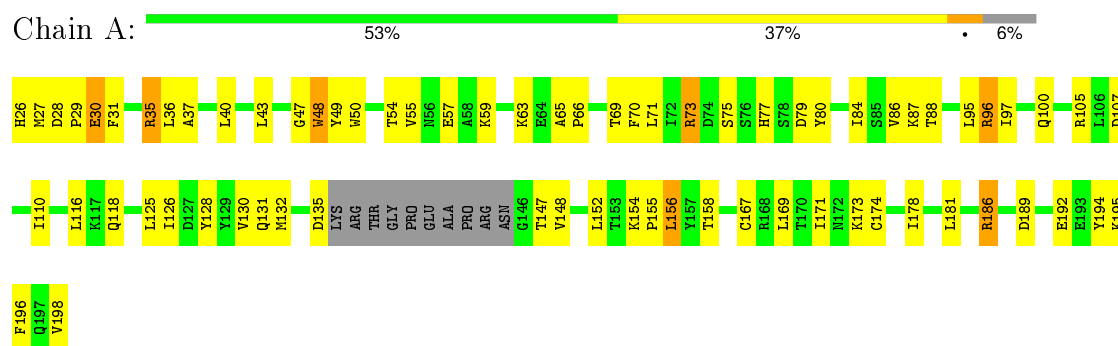
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	341	ARG	VAL	ENGINEERED MUTATION	UNP Q93034
D	345	ASP	LEU	ENGINEERED MUTATION	UNP Q93034
D	387	VAL	-	EXPRESSION TAG	UNP Q93034

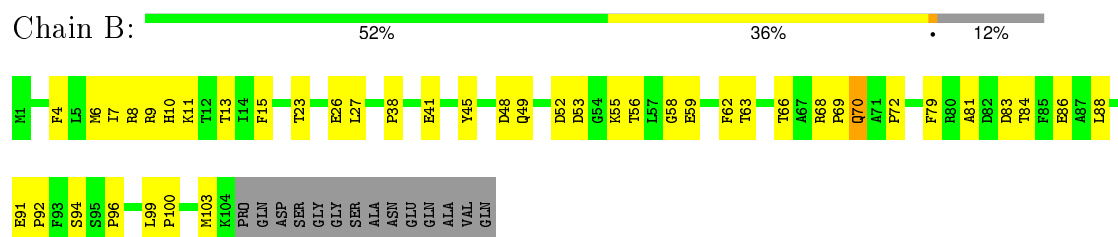
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

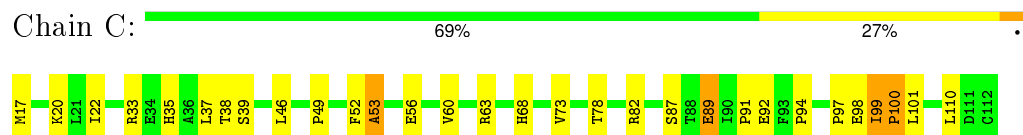
• Molecule 1: Suppressor of cytokine signaling 2



• Molecule 2: Transcription elongation factor B polypeptide 2



• Molecule 3: Transcription elongation factor B polypeptide 1



L354	T276	V180
V355	L277	R181
	L278	
Q360	A279	V185
	E280	
R364	C381	N190
F365	Q282	P191
L366	G283	E192
T367	M284	D193
A368	L285	K194
	K286	L195
A372	R287	Q196
T373	E288	L197
K374	E289	
A375	T290	N201
V376	E291	
	K292	Y206
	L293	L207
D379	E294	D208
	L295	S209
T382	M296	T210
L385	M300	
E386		Y214
V387	P304	R215
	N305	T216
	G306	Q217
	L307	A218
	E308	P219
	P309	
	M310	L222
	L311	Q223
	K312	V227
	D313	Q228
	L314	N229
	E315	Y230
	E316	M231
	L323	K237
	A324	
	D325	R244
	M326	A245
	I333	Y248
	T334	L249
		E250
	E338	T251
	K339	R252
	Y340	R253
	R341	E254
	E342	C255
	Q343	
	L344	L261
		M262
	L347	E263
	F348	C264
	N349	
	R350	F273
		K274
	V352	E275

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.85Å 141.46Å 182.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 49.54 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.00) 96.8 (49.54-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.248 0.226 , 0.250	Depositor DCC
R_{free} test set	3434 reflections (9.96%)	DCC
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 11.2	EDS
Estimated twinning fraction	0.045 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 34527 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5902	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

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	0.30	0/1340	0.60	1/1812 (0.1%)
2	B	0.30	0/844	0.59	0/1139
3	C	0.31	0/780	0.53	0/1055
4	D	0.29	0/3055	0.52	0/4116
All	All	0.29	0/6019	0.55	1/8122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH1	5.24	122.92	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1310	0	1310	66	0
2	B	828	0	834	31	0
3	C	762	0	751	34	0
4	D	3002	0	2987	137	0
All	All	5902	0	5882	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (257) 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)
4:D:167:ARG:HH12	4:D:210:THR:HA	1.20	1.06
4:D:253:ARG:HH11	4:D:253:ARG:HB2	1.31	0.96
1:A:107:ASP:HB3	1:A:110:ILE:HD13	1.48	0.96
4:D:333:ILE:HG23	4:D:340:TYR:HA	1.56	0.87
4:D:109:LYS:HB2	4:D:110:PRO:HD3	1.54	0.87
2:B:9:ARG:HG2	2:B:10:HIS:H	1.40	0.86
3:C:101:LEU:HD12	3:C:101:LEU:H	1.42	0.84
4:D:181:ARG:HD3	4:D:248:TYR:O	1.79	0.81
4:D:315:GLU:HB2	4:D:372:ALA:HB2	1.63	0.81
4:D:285:ILE:HD11	4:D:314:LEU:HD12	1.64	0.79
3:C:35:HIS:O	3:C:38:THR:HG23	1.83	0.77
1:A:54:THR:HG22	1:A:57:GLU:CG	2.15	0.77
4:D:307:ILE:HD11	4:D:364:ARG:CZ	2.17	0.75
4:D:218:ALA:HB3	4:D:219:PRO:HD3	1.66	0.74
2:B:56:THR:OG1	2:B:59:GLU:HG3	1.89	0.72
1:A:54:THR:HG22	1:A:57:GLU:HG3	1.72	0.72
4:D:308:GLU:N	4:D:309:PRO:HD2	2.05	0.71
4:D:73:ILE:HD12	4:D:142:THR:HG22	1.73	0.70
4:D:185:VAL:HG21	4:D:250:GLU:HG2	1.74	0.69
1:A:40:LEU:HD23	1:A:40:LEU:O	1.92	0.68
4:D:73:ILE:HD12	4:D:142:THR:CG2	2.25	0.67
4:D:280:GLU:O	4:D:284:MET:HG3	1.94	0.67
4:D:32:GLN:HE21	4:D:103:GLN:NE2	1.92	0.67
4:D:190:ASN:HB3	4:D:193:ASP:O	1.94	0.66
4:D:173:ASP:OD1	4:D:175:GLN:HB2	1.95	0.66
4:D:69:ILE:HD12	4:D:138:LEU:HD22	1.77	0.66
4:D:307:ILE:HG22	4:D:310:MET:HE2	1.77	0.66
4:D:13:LEU:HD13	4:D:18:LYS:HE3	1.77	0.66
1:A:80:TYR:CE2	1:A:96:ARG:HG2	2.31	0.66
3:C:99:ILE:N	3:C:100:PRO:CD	2.57	0.66
4:D:32:GLN:HE21	4:D:103:GLN:HE21	1.45	0.65
3:C:100:PRO:HG2	3:C:101:LEU:HD12	1.78	0.65
4:D:54:ASP:HB3	4:D:57:GLY:HA3	1.76	0.65
4:D:253:ARG:HB2	4:D:253:ARG:NH1	2.08	0.64
4:D:152:LYS:HG3	4:D:153:ASN:H	1.64	0.63
4:D:214:TYR:HA	4:D:217:GLN:HB3	1.82	0.61
1:A:28:ASP:HB3	1:A:31:PHE:HB3	1.83	0.61
4:D:348:PHE:HB2	4:D:373:TYR:CE2	2.36	0.61
1:A:167:CYS:O	1:A:171:ILE:HG13	2.01	0.61
4:D:355:VAL:HG11	4:D:366:LEU:HD23	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HG2	1:A:118:GLN:HG2	1.83	0.60
2:B:9:ARG:CG	2:B:10:HIS:H	2.14	0.60
4:D:13:LEU:HD11	4:D:49:ALA:HB1	1.84	0.60
1:A:47:GLY:O	1:A:158:THR:HG22	2.02	0.59
2:B:6:MET:HE3	2:B:15:PHE:CE1	2.37	0.59
3:C:53:ALA:HB3	3:C:56:GLU:HB2	1.85	0.59
1:A:130:VAL:HA	1:A:152:LEU:O	2.02	0.59
4:D:138:LEU:O	4:D:138:LEU:HD23	2.03	0.59
1:A:70:PHE:CZ	1:A:155:PRO:HB3	2.37	0.59
4:D:76:ALA:HB1	4:D:96:GLU:HG2	1.85	0.59
2:B:52:ASP:HB3	2:B:55:LYS:HG2	1.85	0.58
2:B:68:ARG:HB3	2:B:70:GLN:OE1	2.03	0.58
2:B:70:GLN:H	2:B:70:GLN:NE2	2.02	0.57
1:A:155:PRO:HG3	1:A:198:VAL:HG22	1.86	0.57
1:A:147:THR:HG22	1:A:148:VAL:N	2.19	0.57
4:D:374:LYS:HD3	4:D:374:LYS:O	2.04	0.57
3:C:99:ILE:N	3:C:100:PRO:HD3	2.18	0.57
4:D:152:LYS:HG3	4:D:153:ASN:N	2.19	0.57
3:C:53:ALA:HB3	3:C:56:GLU:CB	2.35	0.57
4:D:253:ARG:HG3	4:D:254:GLU:N	2.20	0.57
4:D:197:ILE:O	4:D:201:ASN:HB2	2.04	0.57
4:D:56:LYS:HB2	4:D:60:LYS:HE3	1.86	0.56
1:A:71:LEU:HD12	1:A:71:LEU:C	2.26	0.56
2:B:11:LYS:HG3	2:B:91:GLU:HG3	1.87	0.56
1:A:174:CYS:SG	3:C:97:PRO:HB3	2.45	0.56
4:D:277:ILE:O	4:D:296:MET:HE1	2.06	0.56
1:A:54:THR:CG2	1:A:57:GLU:HG3	2.35	0.56
4:D:308:GLU:N	4:D:309:PRO:CD	2.68	0.56
2:B:103:MET:HE1	3:C:101:LEU:HD11	1.87	0.56
1:A:147:THR:HG22	1:A:148:VAL:H	1.71	0.56
4:D:325:ASP:OD2	4:D:347:LEU:HD21	2.06	0.56
4:D:278:LEU:HD13	4:D:309:PRO:HG3	1.88	0.56
1:A:155:PRO:HG3	1:A:198:VAL:CG2	2.36	0.56
1:A:178:ILE:O	1:A:181:LEU:HG	2.06	0.55
1:A:48:TRP:O	1:A:50:TRP:HD1	1.89	0.55
4:D:284:MET:HE1	4:D:292:LYS:HB3	1.87	0.55
1:A:28:ASP:OD2	1:A:30:GLU:HG3	2.06	0.55
1:A:147:THR:HG22	1:A:148:VAL:HG23	1.89	0.55
4:D:91:LYS:O	4:D:95:VAL:HG23	2.07	0.55
1:A:194:TYR:CE1	1:A:196:PHE:HB2	2.40	0.55
1:A:178:ILE:HD11	1:A:195:LYS:NZ	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:278:LEU:HD21	4:D:300:MET:HG3	1.89	0.55
4:D:386:GLU:N	4:D:386:GLU:OE1	2.40	0.55
1:A:195:LYS:HE2	1:A:195:LYS:HA	1.88	0.54
1:A:80:TYR:CZ	1:A:96:ARG:HG2	2.42	0.54
1:A:28:ASP:CG	1:A:29:PRO:HD2	2.28	0.54
4:D:334:THR:HG23	4:D:382:ILE:HG21	1.90	0.54
4:D:98:ARG:HD2	4:D:175:GLN:OE1	2.07	0.54
2:B:6:MET:HB2	2:B:72:PRO:HB2	1.89	0.54
4:D:31:ARG:HH11	4:D:31:ARG:HG3	1.72	0.54
2:B:103:MET:CE	3:C:101:LEU:HD11	2.38	0.54
3:C:17:MET:CE	3:C:33:ARG:HD3	2.37	0.54
1:A:186:ARG:O	1:A:189:ASP:HB2	2.08	0.54
2:B:45:TYR:CE2	2:B:88:LEU:HB2	2.43	0.54
4:D:90:LEU:HD12	4:D:155:LEU:HD22	1.89	0.54
4:D:372:ALA:O	4:D:375:ALA:HB3	2.07	0.53
4:D:338:GLU:O	4:D:342:GLU:HG3	2.08	0.53
4:D:129:ASN:HD22	4:D:132:ASP:H	1.55	0.53
1:A:69:THR:HG23	1:A:156:LEU:HD13	1.90	0.53
3:C:97:PRO:C	3:C:100:PRO:HD3	2.29	0.53
4:D:117:THR:O	4:D:117:THR:HG22	2.09	0.53
2:B:7:ILE:HD11	2:B:27:LEU:HD11	1.91	0.53
1:A:194:TYR:HE1	1:A:196:PHE:HB2	1.74	0.52
3:C:63:ARG:HD3	4:D:42:ASP:OD1	2.09	0.52
4:D:323:LEU:HD23	4:D:376:VAL:HG13	1.91	0.52
4:D:133:SER:HB3	4:D:136:ARG:HB3	1.90	0.52
2:B:4:PHE:CE2	2:B:69:PRO:HG3	2.45	0.52
4:D:294:HIS:NE2	4:D:360:GLN:OE1	2.42	0.52
1:A:54:THR:HG23	1:A:57:GLU:H	1.74	0.52
1:A:59:LYS:O	1:A:63:LYS:HB2	2.10	0.52
1:A:125:LEU:HD23	1:A:125:LEU:C	2.29	0.52
3:C:22:ILE:N	3:C:22:ILE:HD12	2.25	0.52
3:C:99:ILE:H	3:C:100:PRO:HD3	1.75	0.52
4:D:287:ARG:HB2	4:D:289:GLU:HG3	1.92	0.51
4:D:136:ARG:HH11	4:D:136:ARG:HG3	1.75	0.51
1:A:55:VAL:HA	1:A:73:ARG:NH2	2.25	0.51
4:D:385:LEU:C	4:D:385:LEU:HD12	2.31	0.51
4:D:36:THR:OG1	4:D:39:GLN:HG3	2.11	0.51
1:A:126:ILE:O	1:A:130:VAL:HG23	2.11	0.51
1:A:110:ILE:HD12	1:A:110:ILE:N	2.26	0.50
1:A:54:THR:HG22	1:A:57:GLU:CD	2.32	0.50
4:D:31:ARG:HG2	4:D:72:PHE:CD2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:THR:OG1	2:B:26:GLU:HG3	2.11	0.50
4:D:284:MET:HE2	4:D:292:LYS:HD3	1.92	0.50
2:B:8:ARG:HG2	2:B:13:THR:HG23	1.94	0.50
4:D:148:PHE:O	4:D:150:ASN:N	2.45	0.50
4:D:27:LEU:HD12	4:D:31:ARG:HH12	1.77	0.50
4:D:46:ASP:O	4:D:50:VAL:HG23	2.12	0.50
4:D:227:VAL:O	4:D:231:MET:HG3	2.12	0.50
1:A:69:THR:CG2	1:A:156:LEU:HD13	2.42	0.50
1:A:43:LEU:HD13	1:A:49:TYR:HB2	1.94	0.50
4:D:307:ILE:HD11	4:D:364:ARG:NH1	2.26	0.50
4:D:147:ILE:O	4:D:151:ILE:HG12	2.12	0.50
4:D:12:SER:HB3	4:D:14:GLN:NE2	2.27	0.50
4:D:311:LEU:HD23	4:D:365:PHE:CE1	2.47	0.49
4:D:261:LEU:O	4:D:264:CYS:HB3	2.12	0.49
4:D:167:ARG:NH1	4:D:210:THR:HA	2.05	0.49
1:A:178:ILE:HD11	1:A:195:LYS:HE3	1.94	0.49
3:C:49:PRO:HG2	4:D:40:TRP:CD2	2.46	0.49
2:B:94:SER:O	3:C:68:HIS:HB3	2.12	0.49
1:A:84:ILE:CG1	1:A:97:ILE:HD11	2.43	0.49
1:A:95:LEU:HD22	1:A:110:ILE:HD11	1.95	0.49
4:D:76:ALA:O	4:D:80:VAL:HG23	2.13	0.49
1:A:178:ILE:HD12	1:A:192:GLU:OE2	2.12	0.49
1:A:54:THR:CG2	1:A:57:GLU:H	2.26	0.49
2:B:8:ARG:NH2	2:B:91:GLU:O	2.45	0.49
3:C:82:ARG:NH1	3:C:82:ARG:HB3	2.28	0.49
4:D:116:ILE:O	4:D:116:ILE:HG22	2.13	0.49
1:A:77:HIS:HE1	1:A:79:ASP:OD2	1.95	0.48
4:D:24:PRO:O	4:D:28:LYS:HG3	2.13	0.48
2:B:103:MET:HE2	3:C:101:LEU:HD21	1.96	0.48
1:A:198:VAL:HG22	1:A:198:VAL:OXT	2.14	0.48
3:C:17:MET:HE3	3:C:33:ARG:HD3	1.95	0.48
3:C:73:VAL:HG11	3:C:110:LEU:CD1	2.43	0.48
4:D:343:GLN:HA	4:D:343:GLN:OE1	2.14	0.48
4:D:312:LYS:O	4:D:316:GLU:HB2	2.13	0.48
4:D:278:LEU:HD13	4:D:309:PRO:CG	2.43	0.48
4:D:23:ARG:N	4:D:24:PRO:HD2	2.28	0.48
4:D:16:GLU:H	4:D:16:GLU:CD	2.16	0.48
4:D:253:ARG:HG3	4:D:254:GLU:H	1.79	0.48
4:D:195:LEU:CD1	4:D:255:CYS:HB3	2.44	0.48
1:A:69:THR:HA	1:A:154:LYS:O	2.14	0.48
4:D:23:ARG:HG3	4:D:27:LEU:HD21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:LEU:HD12	4:D:31:ARG:NH1	2.29	0.47
1:A:95:LEU:HD12	1:A:95:LEU:O	2.14	0.47
4:D:307:ILE:HG22	4:D:310:MET:CE	2.41	0.47
4:D:31:ARG:NH1	4:D:31:ARG:HG3	2.30	0.47
2:B:58:GLY:HA2	2:B:62:PHE:O	2.14	0.47
4:D:284:MET:CE	4:D:292:LYS:HD3	2.44	0.47
4:D:117:THR:O	4:D:118:LEU:HD23	2.14	0.47
4:D:350:ARG:O	4:D:353:LYS:HB3	2.15	0.47
4:D:176:LEU:O	4:D:180:VAL:HG23	2.15	0.47
1:A:36:LEU:C	1:A:36:LEU:HD23	2.35	0.47
4:D:129:ASN:ND2	4:D:132:ASP:H	2.12	0.47
4:D:113:GLN:NE2	4:D:113:GLN:HA	2.30	0.47
1:A:87:LYS:HD3	1:A:88:THR:N	2.30	0.47
1:A:169:LEU:O	1:A:173:LYS:HG3	2.14	0.47
2:B:48:ASP:O	2:B:49:GLN:HG2	2.15	0.47
4:D:284:MET:CE	4:D:292:LYS:HB3	2.45	0.46
1:A:178:ILE:HD11	1:A:195:LYS:CE	2.45	0.46
2:B:4:PHE:CD2	2:B:69:PRO:HG3	2.50	0.46
3:C:92:GLU:HG2	3:C:94:PRO:HD3	1.98	0.45
2:B:70:GLN:CD	2:B:70:GLN:H	2.19	0.45
4:D:151:ILE:O	4:D:155:LEU:HG	2.17	0.45
2:B:79:PHE:O	2:B:86:GLU:HG2	2.17	0.45
4:D:14:GLN:HB3	4:D:54:ASP:OD2	2.17	0.45
4:D:273:PHE:O	4:D:277:ILE:HG12	2.16	0.45
4:D:72:PHE:O	4:D:75:GLN:HB2	2.17	0.45
3:C:49:PRO:HG2	4:D:40:TRP:CG	2.52	0.45
3:C:52:PHE:CE1	4:D:37:LYS:HE3	2.52	0.45
4:D:244:ARG:HG3	4:D:245:ALA:N	2.32	0.45
1:A:77:HIS:HB3	1:A:80:TYR:CE1	2.52	0.44
4:D:23:ARG:HG3	4:D:27:LEU:CD2	2.46	0.44
1:A:54:THR:C	1:A:73:ARG:HH21	2.20	0.44
3:C:20:LYS:HG2	3:C:22:ILE:CD1	2.48	0.44
4:D:133:SER:HB3	4:D:136:ARG:CB	2.47	0.44
4:D:290:THR:HG22	4:D:354:LEU:HD12	2.00	0.44
4:D:27:LEU:CD1	4:D:31:ARG:HH12	2.31	0.44
3:C:82:ARG:HB3	3:C:82:ARG:HH11	1.82	0.44
2:B:96:PRO:HB3	3:C:99:ILE:HG22	1.98	0.44
1:A:147:THR:CG2	1:A:148:VAL:H	2.29	0.44
1:A:84:ILE:HG13	1:A:97:ILE:HD11	1.99	0.44
1:A:131:GLN:HE21	1:A:131:GLN:HB3	1.58	0.44
1:A:35:ARG:HB2	1:A:35:ARG:HH11	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:HB2	1:A:105:ARG:HH12	1.83	0.43
4:D:38:GLN:NE2	4:D:42:ASP:OD2	2.51	0.43
2:B:99:LEU:HD12	2:B:100:PRO:HD2	2.00	0.43
1:A:65:ALA:HB1	1:A:66:PRO:HD2	2.00	0.43
3:C:20:LYS:HG2	3:C:22:ILE:HD11	1.99	0.43
2:B:91:GLU:OE2	2:B:92:PRO:HD2	2.18	0.43
4:D:385:LEU:C	4:D:386:GLU:HG3	2.39	0.43
2:B:63:THR:OG1	2:B:66:THR:HG23	2.19	0.43
4:D:66:LYS:HB2	4:D:66:LYS:HE3	1.85	0.43
3:C:100:PRO:HG2	3:C:101:LEU:CD1	2.49	0.42
4:D:130:VAL:HG12	4:D:130:VAL:O	2.19	0.42
3:C:37:LEU:C	3:C:39:SER:H	2.21	0.42
4:D:282:GLN:C	4:D:285:ILE:HG22	2.40	0.42
4:D:206:TYR:CD2	4:D:249:LEU:HD21	2.54	0.42
4:D:192:GLU:O	4:D:193:ASP:HB2	2.19	0.42
4:D:54:ASP:HB3	4:D:57:GLY:CA	2.46	0.42
3:C:37:LEU:C	3:C:39:SER:N	2.72	0.42
4:D:323:LEU:CD2	4:D:376:VAL:HG13	2.50	0.42
3:C:101:LEU:H	3:C:101:LEU:CD1	2.21	0.42
1:A:128:TYR:O	1:A:132:MET:HG2	2.19	0.42
4:D:300:MET:O	4:D:306:GLY:HA3	2.20	0.42
2:B:83:ASP:OD2	2:B:84:THR:N	2.50	0.42
4:D:282:GLN:O	4:D:285:ILE:HG22	2.19	0.42
4:D:374:LYS:C	4:D:374:LYS:HD3	2.40	0.41
4:D:38:GLN:O	4:D:42:ASP:OD2	2.38	0.41
2:B:38:PRO:HG2	2:B:41:GLU:HG3	2.02	0.41
4:D:113:GLN:HE21	4:D:113:GLN:HA	1.84	0.41
1:A:26:HIS:CE1	1:A:27:MET:HG3	2.56	0.41
4:D:94:ILE:HD12	4:D:179:GLY:HA3	2.03	0.41
3:C:46:LEU:HD21	3:C:60:VAL:HG23	2.03	0.41
4:D:107:LEU:N	4:D:108:PRO:CD	2.84	0.41
4:D:109:LYS:HB2	4:D:110:PRO:CD	2.37	0.41
4:D:222:LEU:HD11	4:D:227:VAL:HG22	2.02	0.41
4:D:154:ARG:O	4:D:158:SER:HB2	2.19	0.41
4:D:278:LEU:CD1	4:D:309:PRO:HG3	2.50	0.41
4:D:343:GLN:O	4:D:347:LEU:HG	2.21	0.41
1:A:186:ARG:NH1	4:D:113:GLN:OE1	2.54	0.41
1:A:36:LEU:HD23	1:A:37:ALA:N	2.36	0.41
4:D:284:MET:HA	4:D:289:GLU:OE1	2.21	0.40
4:D:65:LEU:O	4:D:69:ILE:HG13	2.21	0.40
4:D:326:MET:HE2	4:D:344:LEU:HD21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG22	1:A:87:LYS:N	2.35	0.40
4:D:237:LYS:HD2	4:D:237:LYS:HA	1.79	0.40
4:D:70:LEU:CD2	4:D:74:LYS:HE3	2.51	0.40
2:B:100:PRO:HD2	2:B:103:MET:CE	2.51	0.40
4:D:273:PHE:N	4:D:273:PHE:CD2	2.90	0.40
3:C:87:SER:C	3:C:89:GLU:H	2.24	0.40
4:D:304:PRO:O	4:D:305:ASN:HB3	2.21	0.40
4:D:138:LEU:HD23	4:D:138:LEU:C	2.41	0.40
1:A:75:SER:C	1:A:77:HIS:H	2.25	0.40
4:D:231:MET:HG2	4:D:277:ILE:HD12	2.03	0.40
4:D:365:PHE:O	4:D:368:ALA:HB3	2.21	0.40
4:D:261:LEU:HD23	4:D:262:MET:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/173 (92%)	142 (89%)	16 (10%)	1 (1%)	30	72
2	B	102/118 (86%)	93 (91%)	8 (8%)	1 (1%)	19	61
3	C	94/96 (98%)	87 (93%)	3 (3%)	4 (4%)	3	19
4	D	364/378 (96%)	322 (88%)	39 (11%)	3 (1%)	24	66
All	All	719/765 (94%)	644 (90%)	66 (9%)	9 (1%)	15	53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	149	SER
4	D	193	ASP
4	D	19	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	ARG
2	B	81	ALA
3	C	53	ALA
3	C	91	PRO
3	C	99	ILE
3	C	100	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/153 (94%)	136 (95%)	7 (5%)	31	71
2	B	92/102 (90%)	90 (98%)	2 (2%)	60	88
3	C	86/86 (100%)	83 (96%)	3 (4%)	43	80
4	D	329/340 (97%)	308 (94%)	21 (6%)	22	59
All	All	650/681 (95%)	617 (95%)	33 (5%)	29	69

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	35	ARG
1	A	48	TRP
1	A	73	ARG
1	A	116	LEU
1	A	135	ASP
1	A	156	LEU
2	B	53	ASP
2	B	70	GLN
3	C	78	THR
3	C	89	GLU
3	C	98	GLU
4	D	13	LEU
4	D	65	LEU
4	D	70	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	86	ASP
4	D	114	LEU
4	D	136	ARG
4	D	208	ASP
4	D	215	ARG
4	D	223	GLN
4	D	229	ASN
4	D	250	GLU
4	D	252	ARG
4	D	253	ARG
4	D	254	GLU
4	D	261	LEU
4	D	275	GLU
4	D	308	GLU
4	D	313	ASP
4	D	325	ASP
4	D	379	ASP
4	D	386	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	124	HIS
1	A	131	GLN
1	A	164	GLN
2	B	70	GLN
3	C	35	HIS
3	C	51	GLN
3	C	108	ASN
4	D	48	HIS
4	D	103	GLN
4	D	129	ASN
4	D	153	ASN
4	D	223	GLN
4	D	229	ASN
4	D	288	ASN
4	D	360	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	163/173 (94%)	-0.18	0 100 100	49, 72, 101, 131	0
2	B	104/118 (88%)	-0.18	0 100 100	44, 62, 89, 98	0
3	C	96/96 (100%)	-0.21	0 100 100	45, 60, 89, 94	0
4	D	368/378 (97%)	-0.22	0 100 100	51, 78, 103, 124	0
All	All	731/765 (95%)	-0.20	0 100 100	44, 73, 100, 131	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.