Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:28 PM GMT

PDB ID	:	5BO4
Title	:	Structure of SOCS2:Elongin C:Elongin B from DMSO-treated crystals
Authors	:	Gadd, M.S.; Bulatov, E.; Ciulli, A.
Deposited on	:	2015-05-27
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

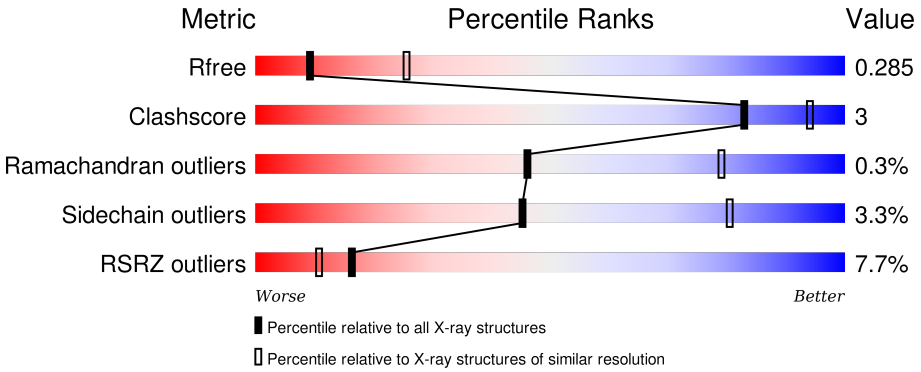
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 <=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	169	2% 79% 12% 9%
1	D	169	9% 83% 7% 9%
1	G	169	% 82% 8% 9%
1	J	169	8% 85% 5% 9%
1	M	169	2% 82% 8% 9%

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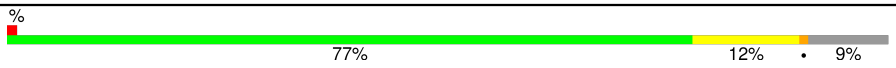
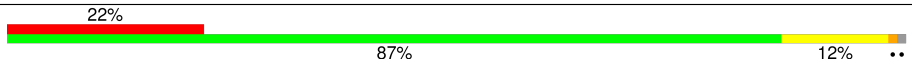
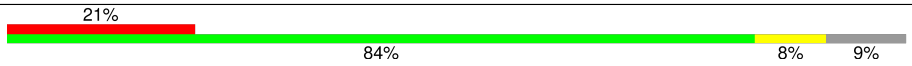
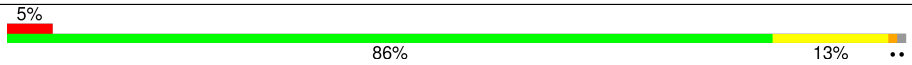
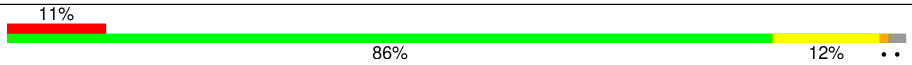
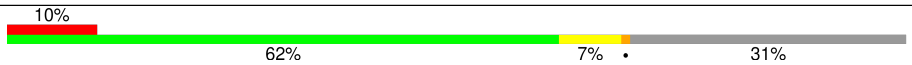
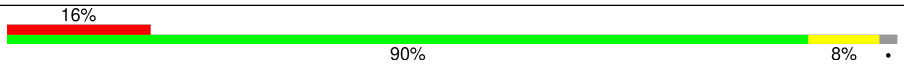
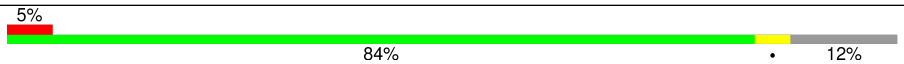
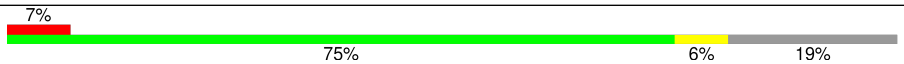
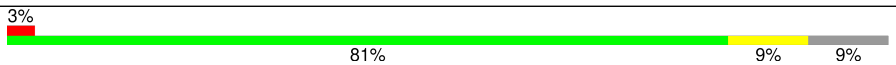
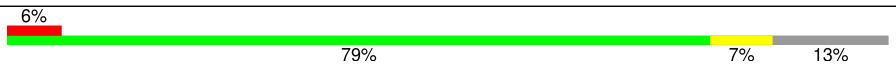
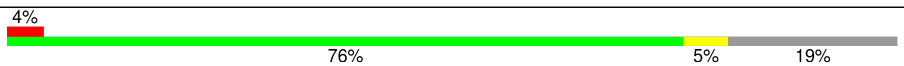
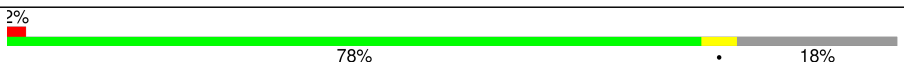
Mol	Chain	Length	Quality of chain
1	P	169	
2	B	104	
2	E	104	
2	H	104	
2	K	104	
2	N	104	
2	Q	104	
3	C	97	
3	F	97	
3	I	97	
3	L	97	
3	O	97	
3	R	97	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14904 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	154	Total	As	C	N	O	S	0	0	0
			1204	1	778	200	218	7			
1	D	154	Total	As	C	N	O	S	0	0	0
			1164	1	752	188	218	5			
1	G	154	Total	As	C	N	O	S	0	0	0
			1189	1	770	194	218	6			
1	J	154	Total	As	C	N	O	S	0	0	0
			1167	1	757	185	218	6			
1	M	153	Total	As	C	N	O	S	0	0	0
			1178	1	764	192	215	6			
1	P	153	Total	As	C	N	O	S	0	0	0
			1192	1	771	194	220	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	expression tag	UNP O14508
A	31	MET	-	expression tag	UNP O14508
D	30	SER	-	expression tag	UNP O14508
D	31	MET	-	expression tag	UNP O14508
G	30	SER	-	expression tag	UNP O14508
G	31	MET	-	expression tag	UNP O14508
J	30	SER	-	expression tag	UNP O14508
J	31	MET	-	expression tag	UNP O14508
M	30	SER	-	expression tag	UNP O14508
M	31	MET	-	expression tag	UNP O14508
P	30	SER	-	expression tag	UNP O14508
P	31	MET	-	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	103	Total	As	C	N	O	S	0	0	0
			693	1	439	113	136	4			
2	E	95	Total	As	C	N	O	S	0	0	0
			709	1	448	120	137	3			
2	H	103	Total	As	C	N	O	S	0	0	0
			743	1	476	123	139	4			
2	K	102	Total	As	C	N	O	S	0	0	0
			755	1	481	125	144	4			
2	N	72	Total		C	N	O	S	0	0	0
			469		291	83	93	2			
2	Q	102	Total	As	C	N	O	S	0	0	0
			730	1	463	124	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	85	Total	C	N	O	S	0	0	0
			633	412	99	117	5			
3	F	79	Total	C	N	O	S	0	0	0
			578	382	89	102	5			
3	I	88	Total	C	N	O	S	0	0	0
			669	435	105	122	7			
3	L	84	Total	C	N	O	S	0	0	0
			619	405	98	111	5			
3	O	79	Total	C	N	O	S	0	0	0
			573	376	89	103	5			
3	R	80	Total	C	N	O	S	0	0	0
			606	400	91	109	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369
F	16	MET	-	initiating methionine	UNP Q15369
I	16	MET	-	initiating methionine	UNP Q15369
L	16	MET	-	initiating methionine	UNP Q15369
O	16	MET	-	initiating methionine	UNP Q15369
R	16	MET	-	initiating methionine	UNP Q15369

- Molecule 4 is water.

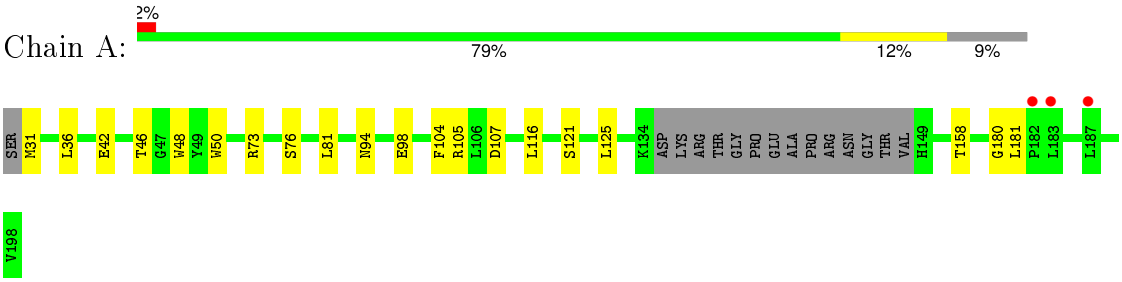
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	D	6	Total O 6 6	0	0
4	F	1	Total O 1 1	0	0
4	G	4	Total O 4 4	0	0
4	I	1	Total O 1 1	0	0
4	J	3	Total O 3 3	0	0
4	M	3	Total O 3 3	0	0
4	P	6	Total O 6 6	0	0
4	R	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

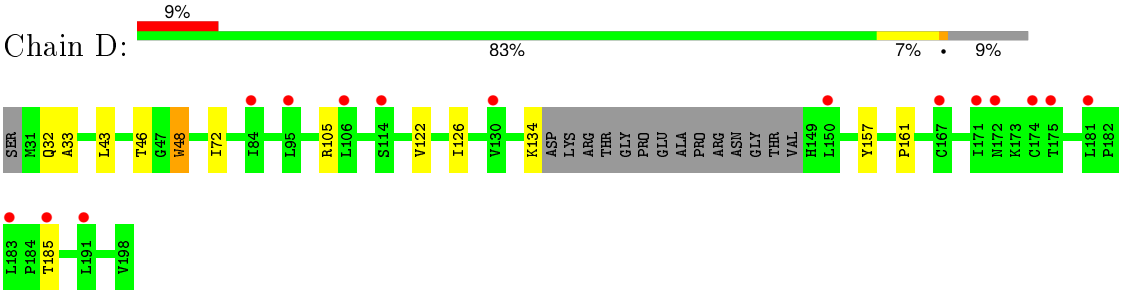
- Molecule 1: Suppressor of cytokine signaling 2

Chain A:



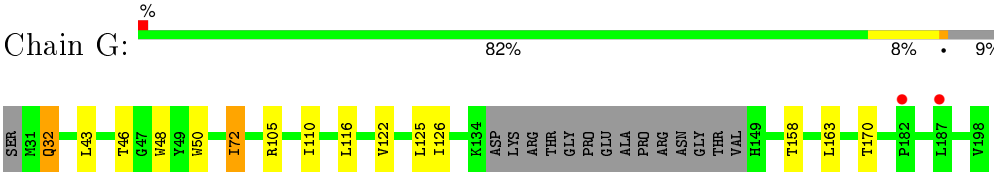
- Molecule 1: Suppressor of cytokine signaling 2

Chain D:



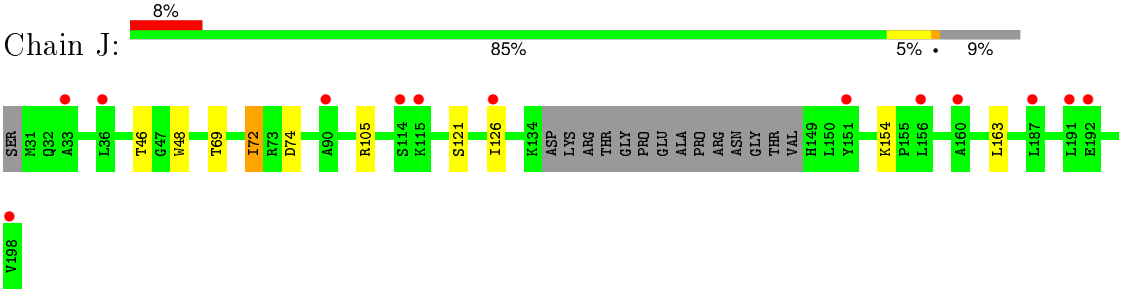
- Molecule 1: Suppressor of cytokine signaling 2

Chain G:



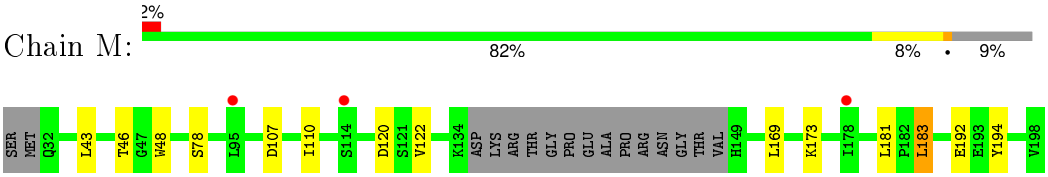
- Molecule 1: Suppressor of cytokine signaling 2

Chain J:



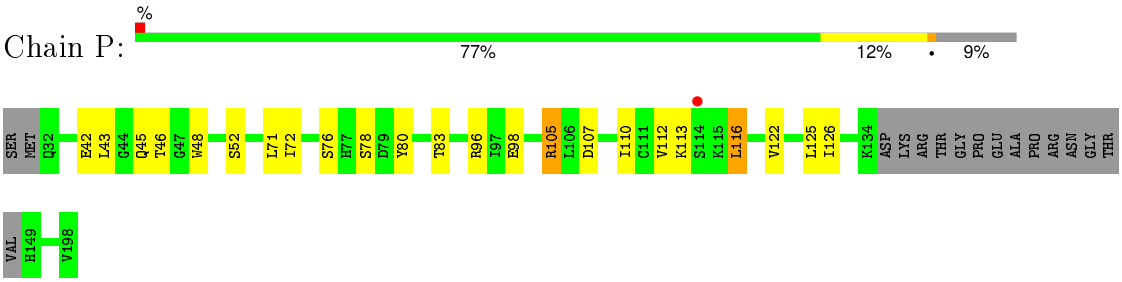
• Molecule 1: Suppressor of cytokine signaling 2

Chain M:



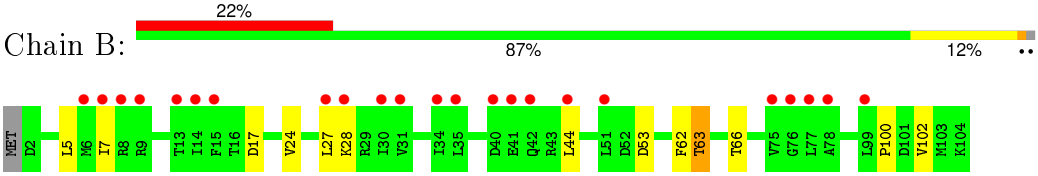
• Molecule 1: Suppressor of cytokine signaling 2

Chain P:



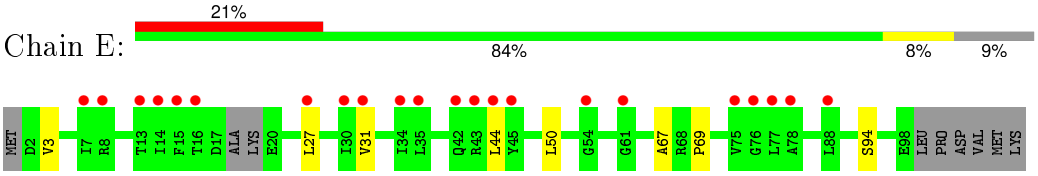
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



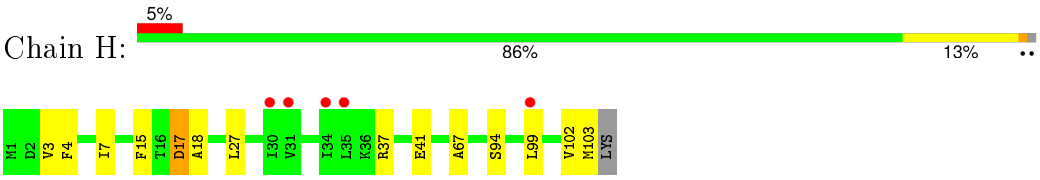
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain E:



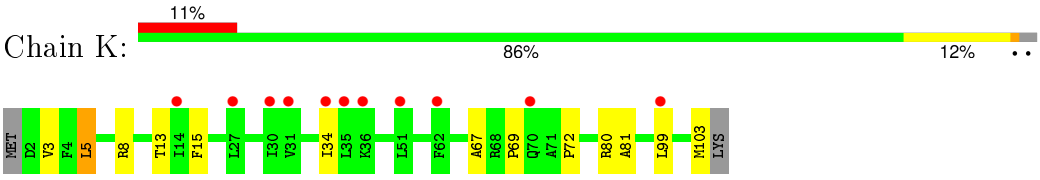
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain H:



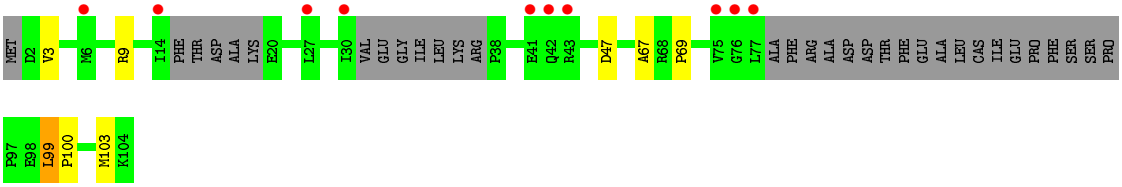
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain K:

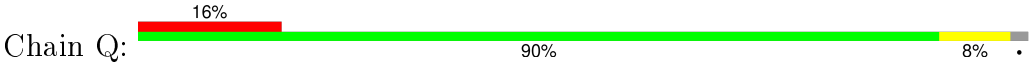


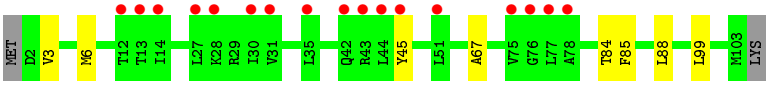
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain N:

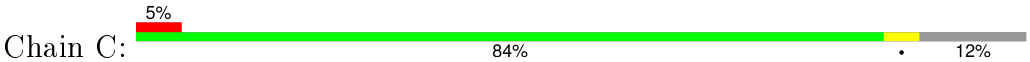


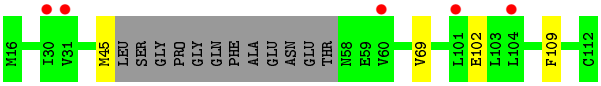
• Molecule 2: Transcription elongation factor B polypeptide 2



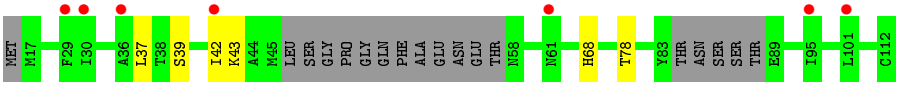


• Molecule 3: Transcription elongation factor B polypeptide 1

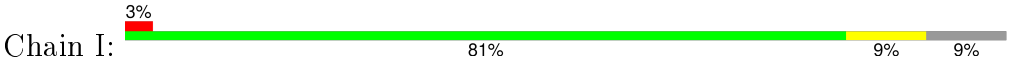


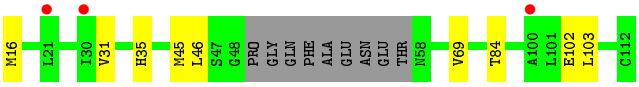


• Molecule 3: Transcription elongation factor B polypeptide 1

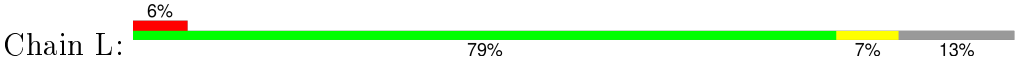


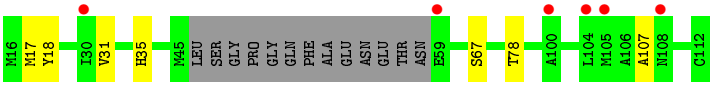
• Molecule 3: Transcription elongation factor B polypeptide 1



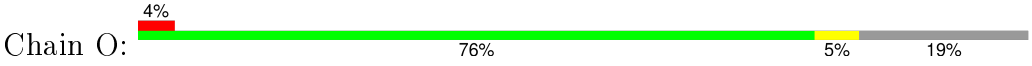


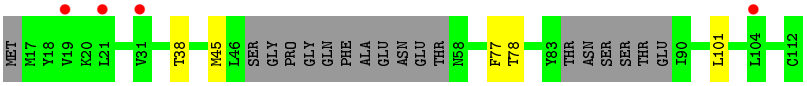
• Molecule 3: Transcription elongation factor B polypeptide 1





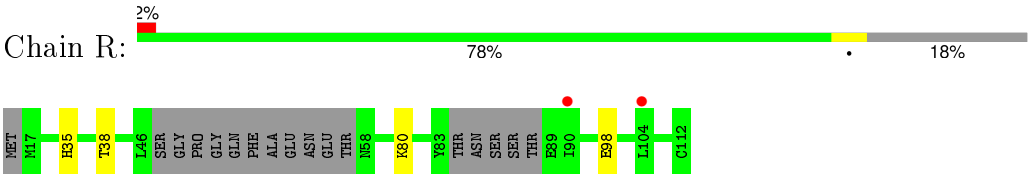
• Molecule 3: Transcription elongation factor B polypeptide 1





• Molecule 3: Transcription elongation factor B polypeptide 1

Chain R:


2%
78%
18%
MET
M17
H35
T38
L46
SER
GLY
PRO
GLY
GLN
PHE
ALA
GLU
ASN
GLU
THR
N58
K80
Y83
THR
ASN
SER
SER
THR
E89
I90
E98
L104
C112

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	185.22Å 185.22Å 67.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.30 – 2.90 45.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.30-2.90) 99.2 (45.02-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.287 0.230 , 0.285	Depositor DCC
R_{free} test set	2862 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	66.0	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.1	EDS
Estimated twinning fraction	0.049 for -h,-k,l 0.053 for h,-h-k,-l 0.259 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 56674 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14904	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.34	0/1221	0.54	0/1656
1	D	0.30	0/1180	0.50	0/1610
1	G	0.39	0/1205	0.59	0/1637
1	J	0.33	0/1183	0.51	0/1613
1	M	0.33	0/1194	0.55	0/1623
1	P	0.39	0/1208	0.58	0/1639
2	B	0.32	0/695	0.50	0/956
2	E	0.34	0/712	0.53	0/967
2	H	0.32	0/749	0.52	0/1024
2	K	0.31	0/760	0.53	0/1035
2	N	0.33	0/472	0.48	0/643
2	Q	0.31	0/734	0.50	0/1002
3	C	0.31	0/647	0.48	0/881
3	F	0.28	0/590	0.44	0/802
3	I	0.33	0/683	0.52	0/924
3	L	0.31	0/633	0.45	0/862
3	O	0.30	0/585	0.45	0/796
3	R	0.32	0/619	0.47	0/837
All	All	0.33	0/15070	0.52	0/20507

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

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	1204	0	1176	11	0
1	D	1164	0	1086	7	0
1	G	1189	0	1148	7	0
1	J	1167	0	1098	6	0
1	M	1178	0	1135	7	0
1	P	1192	0	1162	11	0
2	B	693	0	610	8	0
2	E	709	0	660	5	0
2	H	743	0	684	8	0
2	K	755	0	715	9	0
2	N	469	0	399	4	0
2	Q	730	0	673	3	0
3	C	633	0	594	1	0
3	F	578	0	543	4	0
3	I	669	0	651	4	0
3	L	619	0	572	4	0
3	O	573	0	528	4	0
3	R	606	0	575	2	0
4	A	8	0	0	0	0
4	D	6	0	0	0	0
4	F	1	0	0	0	0
4	G	4	0	0	0	0
4	I	1	0	0	0	0
4	J	3	0	0	0	0
4	M	3	0	0	0	0
4	P	6	0	0	0	0
4	R	1	0	0	0	0
All	All	14904	0	14009	90	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 3.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:VAL:HG23	2:H:67:ALA:HB3	1.75	0.67
2:H:102:VAL:HG23	2:H:103:MET:HG3	1.78	0.66
1:G:46:THR:HB	1:G:48:TRP:CE2	2.32	0.65
2:H:3:VAL:CG2	2:H:67:ALA:HB3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:99:LEU:HD22	2:K:103:MET:HB2	1.82	0.61
2:H:7:ILE:HD11	2:H:27:LEU:HD11	1.82	0.61
1:P:72:ILE:HD11	1:P:126:ILE:HD11	1.85	0.58
1:A:46:THR:HB	1:A:48:TRP:CE2	2.38	0.58
1:M:181:LEU:HD22	3:O:101:LEU:HD21	1.87	0.57
2:B:62:PHE:O	2:B:63:THR:O	2.24	0.56
1:D:43:LEU:HD13	1:D:122:VAL:HG13	1.87	0.56
2:K:15:PHE:HB2	3:L:31:VAL:HG12	1.87	0.56
1:P:43:LEU:HD13	1:P:122:VAL:HG13	1.86	0.56
1:P:43:LEU:HD21	1:P:72:ILE:HG21	1.87	0.56
1:A:36:LEU:HD11	1:A:81:LEU:HD21	1.89	0.54
1:A:181:LEU:HD23	2:B:102:VAL:HG21	1.88	0.54
2:B:100:PRO:HB2	2:B:102:VAL:HG22	1.91	0.52
3:F:37:LEU:HD22	3:F:43:LYS:HA	1.91	0.52
2:K:69:PRO:HB3	3:L:78:THR:HG22	1.90	0.52
1:P:43:LEU:HD22	1:P:122:VAL:HG11	1.91	0.52
1:P:71:LEU:C	1:P:71:LEU:HD12	2.29	0.52
1:D:46:THR:HB	1:D:48:TRP:CE2	2.45	0.52
2:Q:3:VAL:CG2	2:Q:67:ALA:HB3	2.40	0.51
1:D:72:ILE:HD11	1:D:126:ILE:HD11	1.92	0.51
2:Q:45:TYR:CG	2:Q:88:LEU:HD22	2.45	0.51
1:J:46:THR:HB	1:J:48:TRP:CE2	2.46	0.51
1:A:73:ARG:NH2	1:A:94:ASN:OD1	2.43	0.51
2:E:94:SER:O	3:F:68:HIS:HB3	2.10	0.51
1:A:180:GLY:O	2:B:102:VAL:HG11	2.12	0.50
2:N:99:LEU:HD23	2:N:100:PRO:HD2	1.94	0.50
2:K:5:LEU:HA	2:K:72:PRO:HB2	1.94	0.49
2:N:99:LEU:HD22	2:N:103:MET:HB2	1.93	0.49
2:H:15:PHE:HB2	3:I:31:VAL:HG12	1.94	0.49
2:B:63:THR:OG1	2:B:66:THR:HG22	2.12	0.49
1:A:50:TRP:CD2	1:A:158:THR:HG22	2.48	0.49
2:K:8:ARG:HG2	2:K:13:THR:HG23	1.94	0.49
1:G:43:LEU:HD13	1:G:122:VAL:HG13	1.94	0.49
1:P:46:THR:HB	1:P:48:TRP:CE2	2.47	0.48
1:J:72:ILE:HD11	1:J:126:ILE:HD11	1.95	0.48
2:H:37:ARG:NH1	2:H:41:GLU:OE1	2.46	0.48
1:D:33:ALA:HB3	1:J:74:ASP:OD1	2.14	0.48
3:I:45:MET:O	3:I:46:LEU:HD22	2.14	0.48
1:M:43:LEU:HD13	1:M:122:VAL:HG13	1.96	0.47
1:G:50:TRP:CD2	1:G:158:THR:HG22	2.50	0.47
3:O:38:THR:HB	3:O:77:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:LEU:O	2:E:31:VAL:HG23	2.15	0.46
3:R:98:GLU:N	3:R:98:GLU:OE1	2.49	0.46
2:B:28:LYS:HG3	2:B:44:LEU:HD11	1.97	0.46
1:M:183:LEU:HD11	3:O:101:LEU:HD22	1.97	0.45
1:P:98:GLU:OE1	1:P:105:ARG:NH1	2.48	0.45
1:P:113:LYS:HA	1:P:116:LEU:HD22	1.97	0.45
2:K:3:VAL:HG23	2:K:67:ALA:HB3	1.98	0.45
1:A:42:GLU:OE1	1:A:121:SER:OG	2.26	0.45
2:B:7:ILE:HD11	2:B:27:LEU:HD11	1.97	0.45
1:A:46:THR:HB	1:A:48:TRP:NE1	2.31	0.45
2:H:4:PHE:CD2	2:H:17:ASP:HB3	2.52	0.44
2:K:3:VAL:CG2	2:K:67:ALA:HB3	2.48	0.44
1:J:69:THR:HA	1:J:154:LYS:O	2.17	0.44
1:G:72:ILE:HD11	1:G:126:ILE:HD11	1.99	0.44
1:G:163:LEU:HD21	3:I:103:LEU:HD11	2.00	0.44
2:N:69:PRO:HB3	3:O:78:THR:HG22	1.99	0.44
1:G:125:LEU:C	1:G:125:LEU:HD23	2.38	0.44
3:C:69:VAL:HG21	3:C:102:GLU:HB3	2.00	0.44
2:E:69:PRO:HB3	3:F:78:THR:HG22	2.00	0.44
1:A:50:TRP:CE2	1:A:158:THR:HG22	2.54	0.43
1:M:46:THR:HB	1:M:48:TRP:CE2	2.53	0.43
2:E:44:LEU:O	2:E:50:LEU:HD12	2.18	0.43
2:N:3:VAL:HG23	2:N:67:ALA:HB3	2.01	0.43
1:P:125:LEU:HD23	1:P:125:LEU:C	2.39	0.43
3:I:69:VAL:HG21	3:I:102:GLU:HB3	2.01	0.43
1:P:80:TYR:CD1	1:P:96:ARG:HD3	2.53	0.43
1:P:42:GLU:HA	1:P:45:GLN:HE21	1.84	0.42
2:H:3:VAL:HG12	2:H:18:ALA:O	2.19	0.42
1:D:43:LEU:HD21	1:D:72:ILE:HG21	2.02	0.42
2:Q:84:THR:OG1	2:Q:85:PHE:N	2.53	0.42
1:A:98:GLU:O	1:A:104:PHE:HA	2.20	0.42
1:J:163:LEU:HD23	3:L:107:ALA:HB2	2.01	0.42
2:E:3:VAL:CG2	2:E:67:ALA:HB3	2.49	0.41
2:B:24:VAL:HB	2:B:53:ASP:HA	2.02	0.41
1:A:125:LEU:C	1:A:125:LEU:HD23	2.41	0.41
1:M:46:THR:HG22	1:M:194:TYR:OH	2.20	0.41
1:D:157:TYR:CE2	1:D:161:PRO:HG3	2.55	0.41
3:R:38:THR:HG23	3:R:80:LYS:HE2	2.02	0.41
1:M:107:ASP:OD2	1:M:110:ILE:HD13	2.21	0.41
1:G:32:GLN:HE21	1:G:32:GLN:HB3	1.72	0.41
3:F:39:SER:HB3	3:F:42:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ALA:HB3	1:J:74:ASP:CG	2.42	0.40
2:K:34:ILE:HD11	3:L:18:TYR:CZ	2.57	0.40
1:M:169:LEU:O	1:M:173:LYS:HG3	2.21	0.40
2:K:80:ARG:HG2	2:K:81:ALA:N	2.37	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	149/169 (88%)	140 (94%)	8 (5%)	1 (1%)	26 63
1	D	149/169 (88%)	140 (94%)	9 (6%)	0	100 100
1	G	149/169 (88%)	144 (97%)	5 (3%)	0	100 100
1	J	149/169 (88%)	142 (95%)	7 (5%)	0	100 100
1	M	148/169 (88%)	142 (96%)	6 (4%)	0	100 100
1	P	148/169 (88%)	135 (91%)	11 (7%)	2 (1%)	14 44
2	B	100/104 (96%)	91 (91%)	8 (8%)	1 (1%)	19 54
2	E	90/104 (86%)	84 (93%)	6 (7%)	0	100 100
2	H	100/104 (96%)	91 (91%)	9 (9%)	0	100 100
2	K	99/104 (95%)	93 (94%)	6 (6%)	0	100 100
2	N	64/104 (62%)	59 (92%)	4 (6%)	1 (2%)	12 40
2	Q	99/104 (95%)	92 (93%)	7 (7%)	0	100 100
3	C	81/97 (84%)	78 (96%)	3 (4%)	0	100 100
3	F	73/97 (75%)	71 (97%)	2 (3%)	0	100 100
3	I	84/97 (87%)	78 (93%)	6 (7%)	0	100 100
3	L	80/97 (82%)	77 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	O	73/97 (75%)	71 (97%)	2 (3%)	0	100 100
3	R	74/97 (76%)	68 (92%)	6 (8%)	0	100 100
All	All	1909/2220 (86%)	1796 (94%)	108 (6%)	5 (0%)	46 79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	63	THR
1	P	112	VAL
1	A	107	ASP
1	P	107	ASP
2	N	47	ASP

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	124/148 (84%)	120 (97%)	4 (3%)	46 81
1	D	114/148 (77%)	109 (96%)	5 (4%)	35 70
1	G	120/148 (81%)	114 (95%)	6 (5%)	30 65
1	J	115/148 (78%)	112 (97%)	3 (3%)	54 85
1	M	118/148 (80%)	114 (97%)	4 (3%)	44 79
1	P	123/148 (83%)	116 (94%)	7 (6%)	25 59
2	B	62/91 (68%)	60 (97%)	2 (3%)	46 81
2	E	71/91 (78%)	71 (100%)	0	100 100
2	H	71/91 (78%)	68 (96%)	3 (4%)	36 73
2	K	76/91 (84%)	75 (99%)	1 (1%)	76 94
2	N	40/91 (44%)	38 (95%)	2 (5%)	30 65
2	Q	69/91 (76%)	67 (97%)	2 (3%)	50 83
3	C	65/86 (76%)	63 (97%)	2 (3%)	47 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	56/86 (65%)	56 (100%)	0	100 100
3	I	71/86 (83%)	68 (96%)	3 (4%)	36 73
3	L	60/86 (70%)	57 (95%)	3 (5%)	30 65
3	O	56/86 (65%)	55 (98%)	1 (2%)	66 90
3	R	61/86 (71%)	60 (98%)	1 (2%)	70 91
All	All	1472/1950 (76%)	1423 (97%)	49 (3%)	45 80

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	MET
1	A	76	SER
1	A	105	ARG
1	A	116	LEU
2	B	5	LEU
2	B	17	ASP
3	C	45	MET
3	C	109	PHE
1	D	32	GLN
1	D	48	TRP
1	D	105	ARG
1	D	134	LYS
1	D	185	THR
1	G	32	GLN
1	G	72	ILE
1	G	105	ARG
1	G	110	ILE
1	G	116	LEU
1	G	170	THR
2	H	17	ASP
2	H	94	SER
2	H	99	LEU
3	I	16	MET
3	I	35	HIS
3	I	84	THR
1	J	72	ILE
1	J	105	ARG
1	J	121	SER
2	K	5	LEU
3	L	17	MET

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Mol	Chain	Res	Type
3	L	35	HIS
3	L	67	SER
1	M	78	SER
1	M	120	ASP
1	M	183	LEU
1	M	192	GLU
2	N	9	ARG
2	N	99	LEU
3	O	45	MET
1	P	52	SER
1	P	76	SER
1	P	78	SER
1	P	83	THR
1	P	105	ARG
1	P	110	ILE
1	P	116	LEU
2	Q	6	MET
2	Q	99	LEU
3	R	35	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	118	GLN
2	E	10	HIS
1	G	32	GLN
1	M	32	GLN
1	P	32	GLN
1	P	45	GLN
3	R	61	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CAS	A	111	1	4,8,9	1.04	0	2,9,11	1.56	0
2	CAS	B	89	2	4,8,9	1.09	0	2,9,11	2.00	1 (50%)
1	CAS	D	111	1	4,8,9	1.11	0	2,9,11	1.44	1 (50%)
2	CAS	E	89	2	4,8,9	1.05	0	2,9,11	1.86	0
1	CAS	G	111	1	4,8,9	0.81	0	2,9,11	1.67	1 (50%)
2	CAS	H	89	2	4,8,9	1.02	0	2,9,11	1.63	0
1	CAS	J	111	1	4,8,9	0.97	0	2,9,11	1.56	0
2	CAS	K	89	2	4,8,9	1.01	0	2,9,11	1.76	0
1	CAS	M	111	1	4,8,9	1.11	0	2,9,11	1.37	0
1	CAS	P	111	1	4,8,9	1.00	0	2,9,11	1.21	0
2	CAS	Q	89	2	4,8,9	1.03	0	2,9,11	1.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	A	111	1	-	0/0/7/9	0/0/0/0
2	CAS	B	89	2	-	0/0/7/9	0/0/0/0
1	CAS	D	111	1	-	0/0/7/9	0/0/0/0
2	CAS	E	89	2	-	0/0/7/9	0/0/0/0
1	CAS	G	111	1	-	0/0/7/9	0/0/0/0
2	CAS	H	89	2	-	0/0/7/9	0/0/0/0
1	CAS	J	111	1	-	0/0/7/9	0/0/0/0
2	CAS	K	89	2	-	0/0/7/9	0/0/0/0
1	CAS	M	111	1	-	0/0/7/9	0/0/0/0
1	CAS	P	111	1	-	0/0/7/9	0/0/0/0
2	CAS	Q	89	2	-	0/0/7/9	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	89	CAS	CA-CB-SG	-2.26	106.19	114.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	111	CAS	O-C-CA	-2.24	119.72	125.72
1	D	111	CAS	O-C-CA	-2.03	120.28	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	153/169 (90%)	0.12	3 (1%) 68 64	47, 59, 107, 126	0
1	D	153/169 (90%)	0.53	15 (9%) 10 6	61, 82, 128, 163	0
1	G	153/169 (90%)	-0.04	2 (1%) 79 78	35, 48, 90, 102	0
1	J	153/169 (90%)	0.35	13 (8%) 13 8	55, 78, 120, 135	0
1	M	152/169 (89%)	0.19	3 (1%) 68 64	49, 61, 100, 138	0
1	P	152/169 (89%)	0.02	1 (0%) 89 88	37, 49, 79, 134	0
2	B	102/104 (98%)	0.83	23 (22%) 1 0	74, 111, 144, 152	0
2	E	94/104 (90%)	0.93	22 (23%) 1 0	78, 101, 125, 128	0
2	H	102/104 (98%)	0.34	5 (4%) 33 27	62, 88, 103, 117	0
2	K	101/104 (97%)	0.55	11 (10%) 7 4	70, 93, 116, 133	0
2	N	72/104 (69%)	0.89	10 (13%) 4 2	99, 120, 139, 163	0
2	Q	101/104 (97%)	0.79	17 (16%) 2 1	77, 100, 119, 145	0
3	C	85/97 (87%)	0.30	5 (5%) 26 19	66, 85, 112, 144	0
3	F	79/97 (81%)	0.45	7 (8%) 12 7	77, 100, 125, 132	0
3	I	88/97 (90%)	0.06	3 (3%) 49 41	49, 67, 105, 145	0
3	L	84/97 (86%)	0.30	6 (7%) 19 13	72, 92, 130, 141	0
3	O	79/97 (81%)	0.41	4 (5%) 32 25	74, 98, 121, 133	0
3	R	80/97 (82%)	0.19	2 (2%) 61 55	57, 75, 101, 122	0
All	All	1983/2220 (89%)	0.36	152 (7%) 16 11	35, 83, 125, 163	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	77	LEU	7.2
2	B	77	LEU	7.2
2	N	43	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
1	D	150	LEU	6.9
2	N	41	GLU	6.8
1	D	171	ILE	5.9
2	K	34	ILE	5.5
2	B	42	GLN	5.4
2	Q	76	GLY	5.1
2	Q	27	LEU	5.1
2	N	27	LEU	5.1
3	L	104	LEU	4.9
2	K	62	PHE	4.9
2	K	30	ILE	4.7
2	E	76	GLY	4.5
2	N	77	LEU	4.4
1	J	187	LEU	4.4
2	B	76	GLY	4.3
2	E	30	ILE	4.3
2	N	75	VAL	4.3
1	D	172	ASN	4.3
2	Q	44	LEU	4.2
2	E	8	ARG	4.1
2	H	34	ILE	4.1
2	K	36	LYS	4.0
1	G	187	LEU	4.0
3	C	30	ILE	4.0
2	B	78	ALA	4.0
2	Q	35	LEU	4.0
2	E	7	ILE	3.8
2	Q	51	LEU	3.8
2	B	99	LEU	3.8
2	B	8	ARG	3.8
2	B	31	VAL	3.8
2	E	16	THR	3.8
2	H	35	LEU	3.8
2	Q	31	VAL	3.8
2	B	27	LEU	3.7
2	E	27	LEU	3.7
2	E	35	LEU	3.6
2	K	31	VAL	3.6
2	E	31	VAL	3.5
2	E	14	ILE	3.5
2	K	35	LEU	3.5
2	H	99	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	K	27	LEU	3.5
2	B	35	LEU	3.4
2	B	51	LEU	3.4
2	E	77	LEU	3.4
2	K	51	LEU	3.4
2	E	15	PHE	3.4
2	B	30	ILE	3.4
2	N	6	MET	3.3
2	H	30	ILE	3.3
2	Q	75	VAL	3.3
1	D	106	LEU	3.3
3	C	104	LEU	3.3
1	D	167	CYS	3.2
2	E	34	ILE	3.2
2	B	41	GLU	3.2
2	N	30	ILE	3.2
2	N	14	ILE	3.2
3	F	101	LEU	3.1
2	Q	14	ILE	3.1
1	D	174	CYS	3.0
3	L	30	ILE	3.0
2	B	14	ILE	3.0
3	R	90	ILE	3.0
3	L	105	MET	3.0
2	E	45	TYR	2.9
3	C	60	VAL	2.9
1	J	114	SER	2.9
2	E	88	LEU	2.9
1	D	175	THR	2.9
1	D	183	LEU	2.9
1	A	183	LEU	2.8
2	E	78	ALA	2.8
1	P	114	SER	2.8
3	I	30	ILE	2.8
2	B	9	ARG	2.8
1	A	182	PRO	2.8
3	L	108	ASN	2.8
1	J	126	ILE	2.8
2	Q	12	THR	2.8
2	Q	30	ILE	2.7
1	D	191	LEU	2.7
2	B	44	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	182	PRO	2.7
2	B	40	ASP	2.7
2	E	75	VAL	2.7
1	M	95	LEU	2.6
3	I	21	LEU	2.6
3	O	19	VAL	2.6
2	H	31	VAL	2.6
2	Q	78	ALA	2.6
1	A	187	LEU	2.6
2	Q	45	TYR	2.6
1	J	90	ALA	2.6
2	B	7	ILE	2.6
2	Q	13	THR	2.6
2	N	42	GLN	2.5
1	J	115	LYS	2.5
2	E	44	LEU	2.5
1	D	84	ILE	2.5
2	E	61	GLY	2.5
2	E	42	GLN	2.5
3	F	61	ASN	2.5
3	C	31	VAL	2.5
2	E	13	THR	2.5
2	B	75	VAL	2.5
2	Q	42	GLN	2.5
2	N	76	GLY	2.4
2	B	34	ILE	2.4
3	F	42	ILE	2.4
1	J	191	LEU	2.4
1	D	114	SER	2.4
1	J	156	LEU	2.4
2	E	43	ARG	2.4
3	O	21	LEU	2.4
2	K	70	GLN	2.3
1	M	114	SER	2.3
1	J	192	GLU	2.3
2	B	13	THR	2.3
1	D	95	LEU	2.3
1	D	130	VAL	2.3
2	B	28	LYS	2.3
1	J	151	TYR	2.3
1	J	198	VAL	2.3
1	D	181	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	33	ALA	2.3
3	I	100	ALA	2.3
1	M	178	ILE	2.3
3	C	101	LEU	2.3
3	O	31	VAL	2.2
2	E	54	GLY	2.2
2	Q	43	ARG	2.2
3	F	95	ILE	2.2
3	L	100	ALA	2.2
1	J	160	ALA	2.2
3	F	29	PHE	2.2
2	B	6	MET	2.2
2	K	14	ILE	2.2
3	F	30	ILE	2.2
3	R	104	LEU	2.1
1	J	36	LEU	2.1
2	Q	28	LYS	2.1
3	O	104	LEU	2.1
3	L	59	GLU	2.1
2	K	99	LEU	2.1
1	D	185	THR	2.1
3	F	36	ALA	2.1
2	B	15	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
2	CAS	B	89	9/10	0.87	0.16	-	123,130,141,148	0
2	CAS	Q	89	9/10	0.96	0.17	-	99,104,138,142	0
2	CAS	K	89	9/10	0.97	0.14	-	88,97,141,141	0
1	CAS	P	111	9/10	0.98	0.19	-	50,55,63,65	0
1	CAS	M	111	9/10	0.97	0.20	-	70,72,87,92	0
2	CAS	E	89	9/10	0.91	0.12	-	115,118,142,150	0
1	CAS	D	111	9/10	0.97	0.27	-	77,87,97,99	0
2	CAS	H	89	9/10	0.97	0.14	-	75,82,122,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CAS	A	111	9/10	0.98	0.19	-	61,66,89,98	0
1	CAS	G	111	9/10	0.98	0.23	-	50,58,59,66	0
1	CAS	J	111	9/10	0.97	0.16	-	78,93,101,104	0

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.