



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:13 PM GMT

PDB ID : 1J5E
Title : Structure of the Thermus thermophilus 30S Ribosomal Subunit
Authors : Wimberly, B.T.; Brodersen, D.E.; Clemons Jr., W.M.; Morgan-Warren, R.;
Carter, A.P.; Vornrhein, C.; Hartsch, T.; Ramakrishnan, V.
Deposited on : 2002-04-08
Resolution : 3.05 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

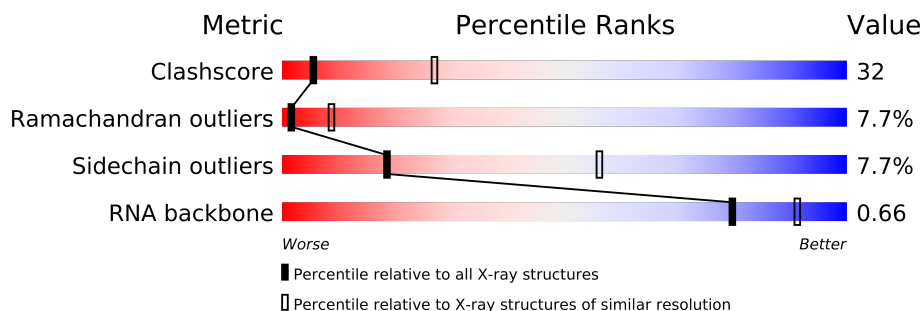
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.05 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))
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RNA backbone	1838	1006 (3.52-2.60)

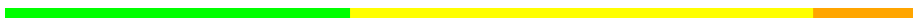
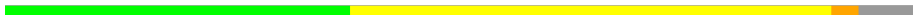
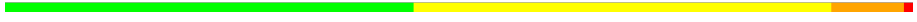

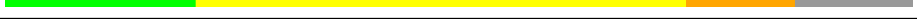


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	208	
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	135	
13	M	126	
14	N	60	

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Mol	Chain	Length	Quality of chain
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51933 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	66	0	0
			32514	14472	6016	10513	1513			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	CONFLICT	EMBL 11125386

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

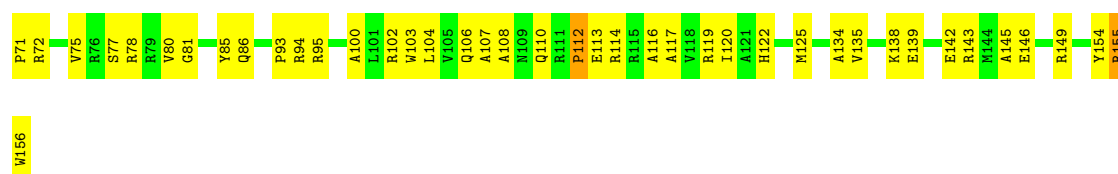
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	D	1	Total	Zn	0	0
			1	1		
22	N	1	Total	Zn	0	0
			1	1		

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	X	0	0
			1	1		
23	A	186	Total	X	0	0
			186	186		
23	M	1	Total	X	0	0
			1	1		

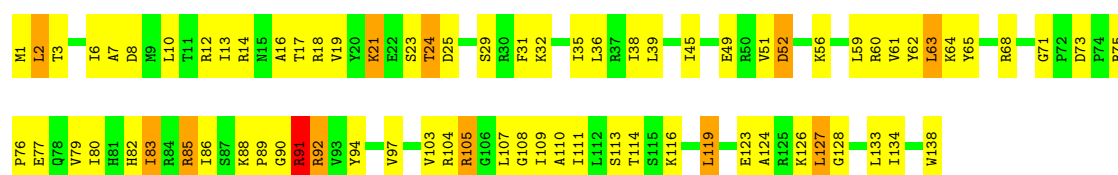






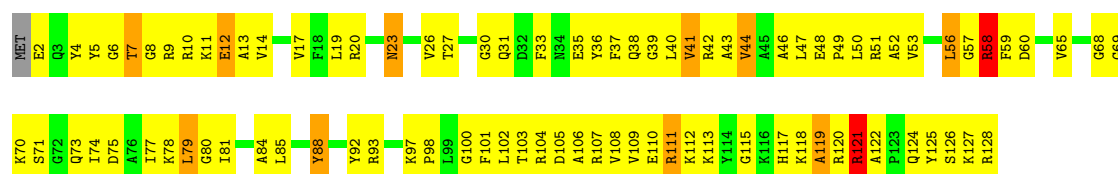
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



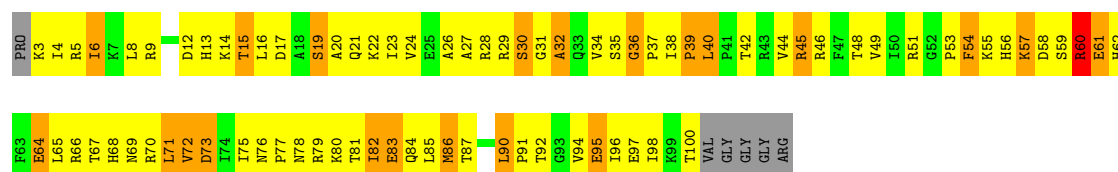
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



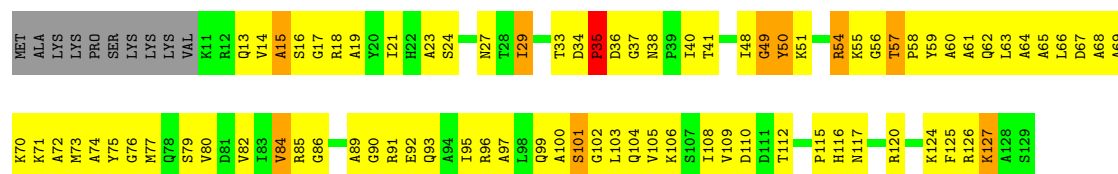
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:



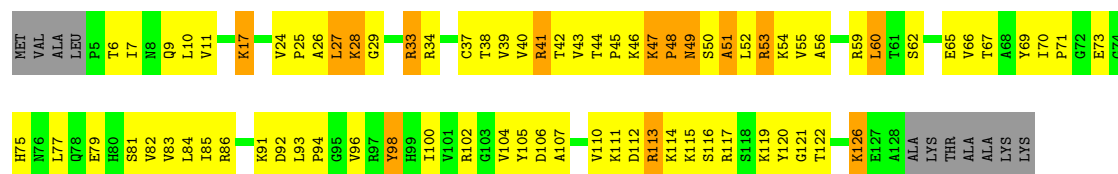
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



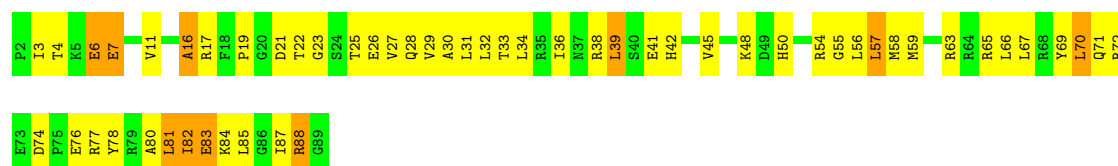
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:



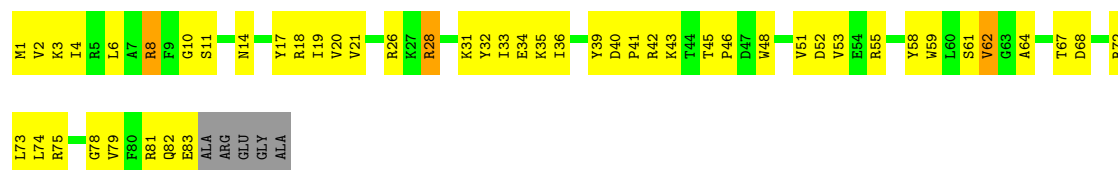
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



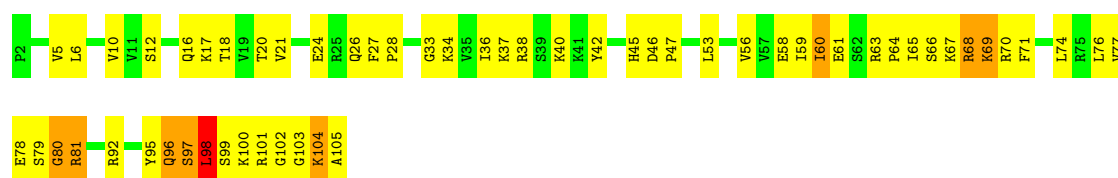
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



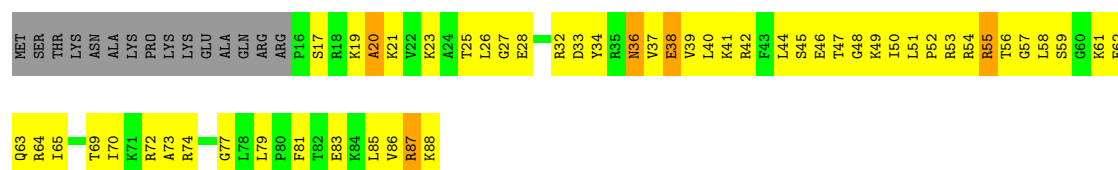
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



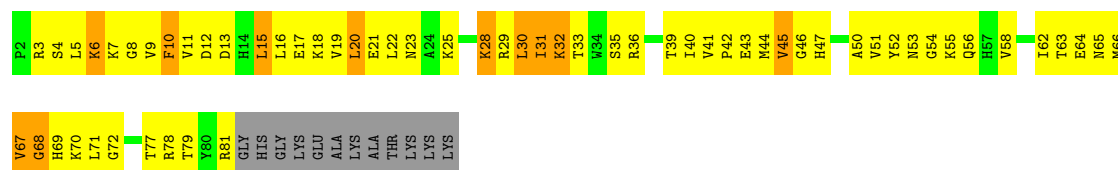
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S: 



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T: 



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain V: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.38Å 401.38Å 175.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.76 – 3.05	Depositor
% Data completeness (in resolution range)	94.0 (59.76-3.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.252	Depositor
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.217	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 254234 reflections	Xtriage
Total number of atoms	51933	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, 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	0.48	0/36393	0.75	41/56797 (0.1%)
2	B	0.36	0/1935	0.67	1/2609 (0.0%)
3	C	0.37	0/1636	0.66	0/2205
4	D	0.37	0/1733	0.63	0/2318
5	E	0.48	0/1162	0.79	0/1564
6	F	0.33	0/856	0.62	0/1154
7	G	0.34	0/1276	0.61	0/1709
8	H	0.44	0/1136	0.74	0/1527
9	I	0.36	0/1029	0.62	0/1378
10	J	0.36	0/805	0.71	0/1082
11	K	0.39	0/900	0.70	0/1213
12	L	0.42	0/986	0.73	0/1320
13	M	0.35	0/1008	0.67	0/1347
14	N	0.40	0/501	0.78	0/664
15	O	0.36	0/745	0.63	1/992 (0.1%)
16	P	0.43	0/716	0.76	0/963
17	Q	0.44	0/870	0.75	0/1159
18	R	0.36	0/603	0.63	0/799
19	S	0.34	0/661	0.72	1/890 (0.1%)
20	T	0.39	0/764	0.73	0/1006
21	V	0.42	0/212	0.64	0/277
All	All	0.45	0/55927	0.73	44/82973 (0.1%)

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	2	40

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.93	131.35	109.50
1	A	243	A	C2'-C3'-O3'	9.45	130.28	109.50
1	A	181	G	C2'-C3'-O3'	9.13	129.59	109.50
1	A	559	A	C2'-C3'-O3'	9.12	129.56	109.50
1	A	1299	A	N9-C1'-C2'	8.59	125.17	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	181	G	C3'
1	A	1528	U	C3'

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	U	Sidechain
1	A	197	A	Sidechain
1	A	203	U	Sidechain
1	A	231	G	Sidechain
1	A	249	U	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32514	0	16410	1113	0
2	B	1900	0	1951	217	1
3	C	1612	0	1677	226	0
4	D	1703	0	1764	146	0
5	E	1146	0	1207	104	0
6	F	843	0	857	72	0
7	G	1257	0	1296	93	0
8	H	1116	0	1177	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1011	0	1043	113	0
10	J	792	0	835	130	0
11	K	885	0	904	85	0
12	L	970	0	1057	118	0
13	M	997	0	1072	121	0
14	N	492	0	529	74	0
15	O	734	0	771	55	0
16	P	700	0	720	56	0
17	Q	857	0	930	84	0
18	R	597	0	668	68	0
19	S	647	0	673	81	0
20	T	762	0	859	78	0
21	V	208	0	221	26	0
22	D	1	0	0	0	0
22	N	1	0	0	0	0
23	A	186	0	0	0	0
23	B	1	0	0	0	0
23	M	1	0	0	0	0
All	All	51933	0	36621	2836	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

The worst 5 of 2836 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:41:ARG:HG2	12:L:42:THR:H	1.03	1.15
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.22	1.14
1:A:1443:G:H5''	1:A:1446:A:H5'	1.28	1.11
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.32	1.09
4:D:36:ARG:H	4:D:37:PRO:HD3	1.19	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:157:ARG:NH1	2:B:157:ARG:NH1[7_555]	1.70	0.50

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	
2	B	232/256 (91%)	174 (75%)	34 (15%)	24 (10%)	1	4
3	C	204/239 (85%)	135 (66%)	40 (20%)	29 (14%)	0	2
4	D	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	4	23
5	E	148/161 (92%)	130 (88%)	13 (9%)	5 (3%)	6	31
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	22	69
7	G	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	2	12
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	7	36
9	I	125/128 (98%)	88 (70%)	27 (22%)	10 (8%)	1	8
10	J	96/104 (92%)	59 (62%)	20 (21%)	17 (18%)	0	0
11	K	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	9
12	L	122/135 (90%)	98 (80%)	15 (12%)	9 (7%)	2	9
13	M	123/126 (98%)	88 (72%)	27 (22%)	8 (6%)	2	12
14	N	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	1	3
15	O	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	3	16
16	P	81/88 (92%)	65 (80%)	15 (18%)	1 (1%)	19	63
17	Q	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	8
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	8	37
19	S	78/92 (85%)	49 (63%)	18 (23%)	11 (14%)	0	2
20	T	97/106 (92%)	65 (67%)	20 (21%)	12 (12%)	1	3
21	V	22/26 (85%)	19 (86%)	2 (9%)	1 (4%)	4	23
All	All	2356/2532 (93%)	1811 (77%)	363 (15%)	182 (8%)	1	9

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS

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Mol	Chain	Res	Type
2	B	17	PHE
2	B	21	ARG

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	
2	B	202/220 (92%)	180 (89%)	22 (11%)	9	35
3	C	160/188 (85%)	142 (89%)	18 (11%)	9	33
4	D	180/180 (100%)	172 (96%)	8 (4%)	39	80
5	E	115/122 (94%)	100 (87%)	15 (13%)	6	25
6	F	90/90 (100%)	88 (98%)	2 (2%)	64	93
7	G	126/126 (100%)	122 (97%)	4 (3%)	51	88
8	H	119/119 (100%)	109 (92%)	10 (8%)	16	51
9	I	98/99 (99%)	90 (92%)	8 (8%)	17	52
10	J	87/91 (96%)	78 (90%)	9 (10%)	10	37
11	K	90/99 (91%)	84 (93%)	6 (7%)	23	63
12	L	104/111 (94%)	96 (92%)	8 (8%)	18	56
13	M	100/101 (99%)	90 (90%)	10 (10%)	11	39
14	N	49/49 (100%)	47 (96%)	2 (4%)	41	83
15	O	79/79 (100%)	72 (91%)	7 (9%)	14	47
16	P	72/74 (97%)	67 (93%)	5 (7%)	22	62
17	Q	96/96 (100%)	90 (94%)	6 (6%)	25	66
18	R	64/77 (83%)	61 (95%)	3 (5%)	36	79
19	S	71/79 (90%)	68 (96%)	3 (4%)	40	82
20	T	76/82 (93%)	69 (91%)	7 (9%)	13	45
21	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1997/2103 (95%)	1844 (92%)	153 (8%)	18	56

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	2	LEU
9	I	111	ARG
18	R	38	GLU
8	H	52	ASP
8	H	105	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	64	GLN
9	I	73	GLN
18	R	36	ASN
6	F	94	GLN
7	G	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1512/1522 (99%)	220 (14%)	88 (5%)

5 of 220 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	976	G
1	A	1397	C
1	A	701	C
1	A	840	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 190 ligands modelled in this entry, 188 are unknown and 2 are 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.