



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:52 AM GMT

PDB ID : 2V3C
Title : CRYSTAL STRUCTURE OF THE SRP54-SRP19-7S.S SRP RNA COM-
PLEX OF M. JANNASCHII
Authors : Hainzl, T.; Huang, S.; Sauer-Eriksson, A.E.
Deposited on : 2007-06-15
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure 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/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

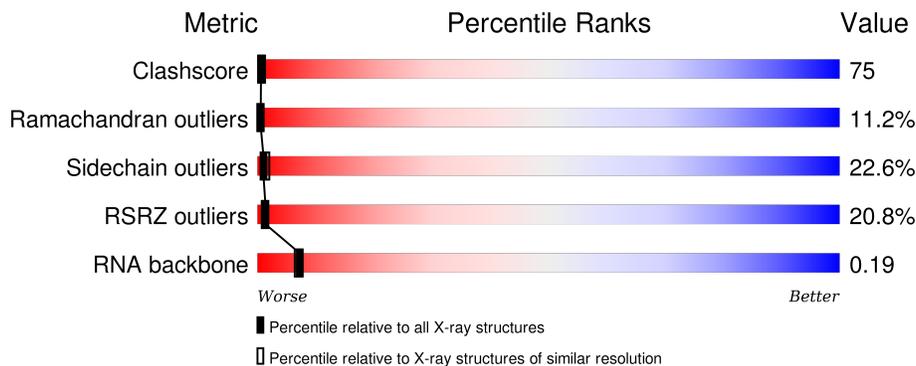
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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	87	
1	B	87	
2	C	432	
2	D	432	
3	M	96	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	N	96	 23% 45% 32%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12336 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 SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	87	727	468	130	125	4	0	0	0
1	B	87	727	468	130	125	4	0	0	0

- Molecule 2 is a protein called SIGNAL RECOGNITION 54 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	404	3149	1998	541	600	10	0	0	1
2	D	402	3133	1989	538	597	9	0	0	1

- Molecule 3 is a RNA chain called 7S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	M	96	2063	919	385	664	95	0	0	0
3	N	96	2063	919	385	664	95	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	26	Total 26	O 26	0	0
4	C	107	Total 107	O 107	0	0
4	D	107	Total 107	O 107	0	0

Continued on next page...

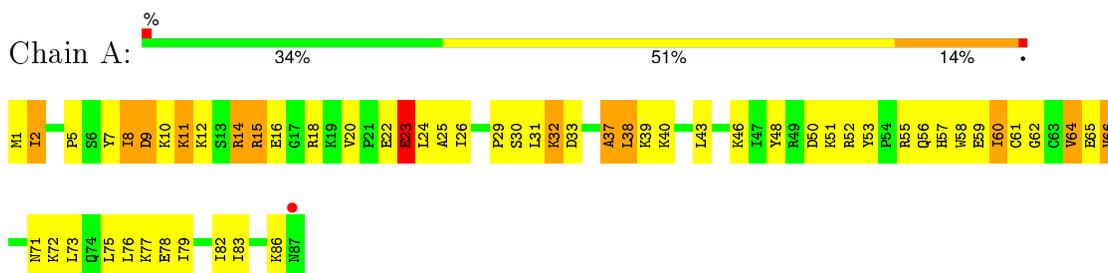
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	92	Total 92	O 92	0	0
4	N	119	Total 119	O 119	0	0

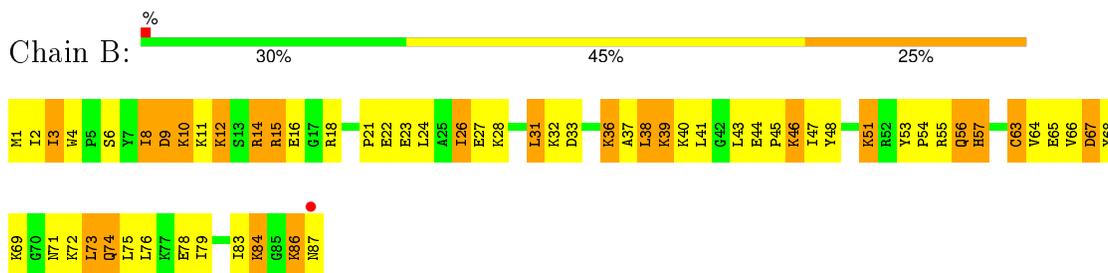
3 Residue-property plots

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.

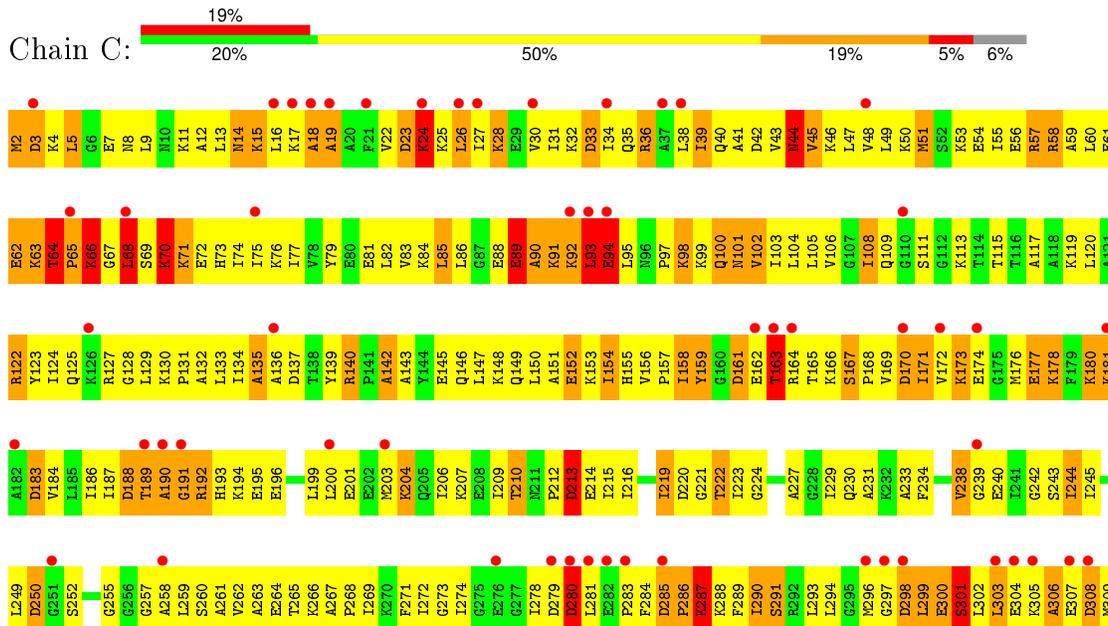
- Molecule 1: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN



- Molecule 1: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN



- Molecule 2: SIGNAL RECOGNITION 54 KDA PROTEIN



G142	G143	C144	G145	G146	U147	G148	G149	G150	G151	G152	A153	G154	C155	A156	U157	C158	U159	C160	C161	U162	G163	U164	A165	G166	G167	G168	G169	A170	G171	A172	U173	G174	U175	A176	A177	G178	C179	C180	C181	C182	U183	U184	U185	A186	C187	C188	U189	G190	C191	C192	G193	A194	A195	C196	C197	C198	C199	G200	G201																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C202	A203	G204	G205	C206	C207	C208	G209	G210	A211	A212	G213	G214	G215	A216	G217	C218	A219	A220	C221	G222	G223	U224	A225	G226	G227	C228	A229	G230	G231	A232	C233	G234	U235	C236	A237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.29Å 129.40Å 163.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 32.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 93.6 (32.35-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.244 , 0.294 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	57.8	Xtrriage
Anisotropy	0.510	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 74.8	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Outliers	2 of 55298 reflections (0.004%)	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12336	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.55% 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

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	1.19	1/740 (0.1%)	1.26	4/984 (0.4%)
1	B	1.15	1/740 (0.1%)	1.17	6/984 (0.6%)
2	C	0.83	1/3176 (0.0%)	1.05	16/4248 (0.4%)
2	D	0.63	0/3160	0.99	16/4227 (0.4%)
3	M	2.58	140/2309 (6.1%)	3.88	600/3603 (16.7%)
3	N	2.26	91/2309 (3.9%)	3.38	476/3603 (13.2%)
All	All	1.62	234/12434 (1.9%)	2.46	1118/17649 (6.3%)

The worst 5 of 234 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	218	C	N1-C6	-14.80	1.28	1.37
3	M	217	G	C8-N7	12.07	1.38	1.30
3	M	217	G	N7-C5	11.67	1.46	1.39
3	M	168	G	N3-C4	-11.48	1.27	1.35
3	N	172	A	N9-C4	11.11	1.44	1.37

The worst 5 of 1118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	209	G	C5-C6-O6	-24.70	113.78	128.60
3	M	194	A	O4'-C1'-N9	-20.43	91.86	108.20
3	M	217	G	C5-C6-O6	-20.20	116.48	128.60
3	N	217	G	C5-C6-O6	-19.78	116.73	128.60
3	M	142	G	O4'-C1'-N9	-18.30	93.56	108.20

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	727	0	786	80	0
1	B	727	0	786	90	0
2	C	3149	0	3364	579	0
2	D	3133	0	3349	620	0
3	M	2063	0	1043	162	0
3	N	2063	0	1041	136	0
4	A	23	0	0	2	0
4	B	26	0	0	2	0
4	C	107	0	0	17	0
4	D	107	0	0	21	0
4	M	92	0	0	11	0
4	N	119	0	0	4	0
All	All	12336	0	10369	1633	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 75.

The worst 5 of 1633 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:D:18:ALA:CB	2:D:71:LYS:HD2	1.54	1.34
2:C:325:LYS:HA	2:C:325:LYS:NZ	1.51	1.21
2:D:18:ALA:HB1	2:D:71:LYS:CD	1.71	1.19
2:D:290:ILE:HG23	2:D:294:LEU:HD21	1.22	1.18
2:C:64:THR:HG22	2:C:66:LYS:HB2	1.25	1.15

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	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	4	6
1	B	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	2	2
2	C	400/432 (93%)	258 (64%)	97 (24%)	45 (11%)	0	0
2	D	398/432 (92%)	227 (57%)	116 (29%)	55 (14%)	0	0
All	All	968/1038 (93%)	621 (64%)	239 (25%)	108 (11%)	0	0

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	18	ALA
2	C	19	ALA
2	C	24	LYS
2	C	64	THR
2	C	68	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	80/80 (100%)	69 (86%)	11 (14%)	4	8
1	B	80/80 (100%)	63 (79%)	17 (21%)	1	2
2	C	340/364 (93%)	264 (78%)	76 (22%)	1	1
2	D	338/364 (93%)	253 (75%)	85 (25%)	1	1
All	All	838/888 (94%)	649 (77%)	189 (23%)	1	1

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	303	LEU
2	D	4	LYS
2	D	327	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	313	LYS
2	C	334	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	334	GLN
2	C	340	ASN
2	D	101	ASN
2	C	329	ASN
2	D	226	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	95/96 (98%)	52 (54%)	16 (16%)
3	N	95/96 (98%)	41 (43%)	7 (7%)
All	All	190/192 (98%)	93 (48%)	23 (12%)

5 of 93 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	M	145	G
3	M	146	G
3	M	147	U
3	M	149	G
3	M	153	A

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	M	181	C
3	M	193	G
3	N	193	G
3	M	185	U
3	M	195	A

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	87/87 (100%)	0.34	1 (1%) 82 84	27, 42, 50, 53	0
1	B	87/87 (100%)	0.27	1 (1%) 82 84	27, 42, 53, 62	0
2	C	404/432 (93%)	1.09	80 (19%) 1 1	29, 57, 77, 88	0
2	D	402/432 (93%)	2.02	161 (40%) 0 0	31, 67, 80, 89	0
3	M	96/96 (100%)	-0.39	1 (1%) 84 86	18, 37, 50, 61	0
3	N	96/96 (100%)	-0.35	0 100 100	20, 37, 52, 70	0
All	All	1172/1230 (95%)	1.05	244 (20%) 1 1	18, 56, 77, 89	0

The worst 5 of 244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	280	ASP	13.6
2	D	251	GLY	13.5
2	D	301	SER	12.4
2	D	141	PRO	12.2
2	C	314	THR	11.3

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

There are no such residues in this entry.