



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:36 PM UTC

PDB ID : 2O61 / pdb_00002o61
Title : Crystal Structure of NFkB, IRF7, IRF3 bound to the interferon-b enhancer
Authors : Panne, D.
Deposited on : 2006-12-06
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

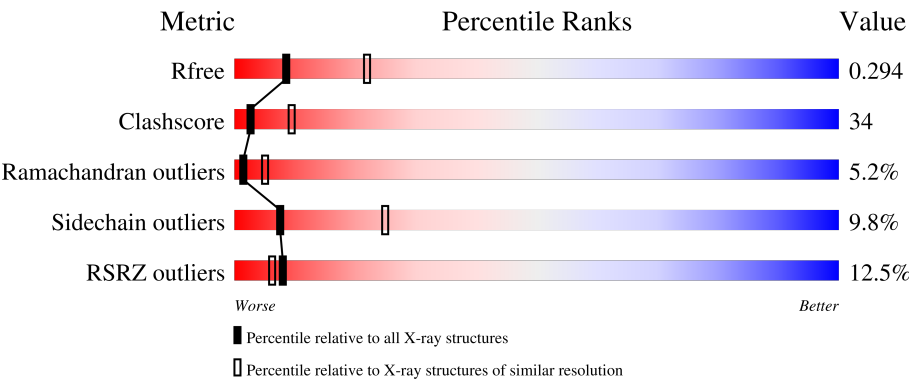
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	E	36	
2	F	34	
3	A	540	
4	B	314	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7912 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 DNA chain called 36-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	36	Total	C	N	O	P	0	0	0
			750	357	147	211	35			

- Molecule 2 is a DNA chain called 34-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	34	Total	C	N	O	P	0	0	0
			678	328	110	207	33			

- Molecule 3 is a protein called Transcription factor p65/Interferon regulatory factor 7/Interferon regulatory factor 3 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	498	Total	C	N	O	S	0	0	0
			3988	2505	745	722	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q04206
A	19	GLY	-	cloning artifact	UNP Q04206
A	292	GLY	-	linker	UNP Q04206
A	293	SER	-	linker	UNP Q04206
A	294	LEU	-	linker	UNP Q04206
A	295	SER	-	linker	UNP Q04206
A	296	SER	-	linker	UNP Q04206
A	297	GLY	-	linker	UNP Q04206
A	298	SER	-	linker	UNP Q04206
A	299	SER	-	linker	UNP Q04206
A	300	LEU	-	linker	UNP Q04206
A	301	SER	-	linker	UNP Q04206
A	302	SER	-	linker	UNP Q04206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	303	PRO	-	linker	UNP Q04206
A	304	SER	-	linker	UNP Q04206
A	305	ALA	-	linker	UNP Q04206
A	306	GLY	-	linker	UNP Q04206
A	1118	GLN	PRO	engineered mutation	UNP Q92985
A	1126	GLY	-	linker	UNP Q92985
A	1127	SER	-	linker	UNP Q92985
A	1128	LEU	-	linker	UNP Q92985
A	1129	SER	-	linker	UNP Q92985
A	1130	SER	-	linker	UNP Q92985
A	1131	ASP	-	linker	UNP Q92985
A	1132	SER	-	linker	UNP Q92985
A	1133	SER	-	linker	UNP Q92985
A	1134	LEU	-	linker	UNP Q92985
A	1135	SER	-	linker	UNP Q92985
A	1136	SER	-	linker	UNP Q92985
A	1137	PRO	-	linker	UNP Q92985
A	1138	SER	-	linker	UNP Q92985
A	1139	ALA	-	linker	UNP Q92985
A	1140	LEU	-	linker	UNP Q92985
A	1141	SER	-	linker	UNP Q92985
A	1142	PRO	-	linker	UNP Q92985
A	1143	LYS	-	linker	UNP Q92985
A	1144	PRO	-	linker	UNP Q92985
A	1145	ARG	-	linker	UNP Q92985
A	1146	ILE	-	linker	UNP Q92985
A	2112	GLY	-	expression tag	UNP Q14653
A	2113	LEU	-	expression tag	UNP Q14653
A	2114	GLU	-	expression tag	UNP Q14653
A	2115	HIS	-	expression tag	UNP Q14653
A	2116	HIS	-	expression tag	UNP Q14653
A	2117	HIS	-	expression tag	UNP Q14653
A	2118	HIS	-	expression tag	UNP Q14653
A	2119	HIS	-	expression tag	UNP Q14653
A	2120	HIS	-	expression tag	UNP Q14653

- Molecule 4 is a protein called Nuclear factor NF-kappa-B p105 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	314	Total	C	N	O	S	0	0	0
			2471	1566	430	462	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	MET	-	initiating methionine	UNP P19838

- Molecule 5 is water.

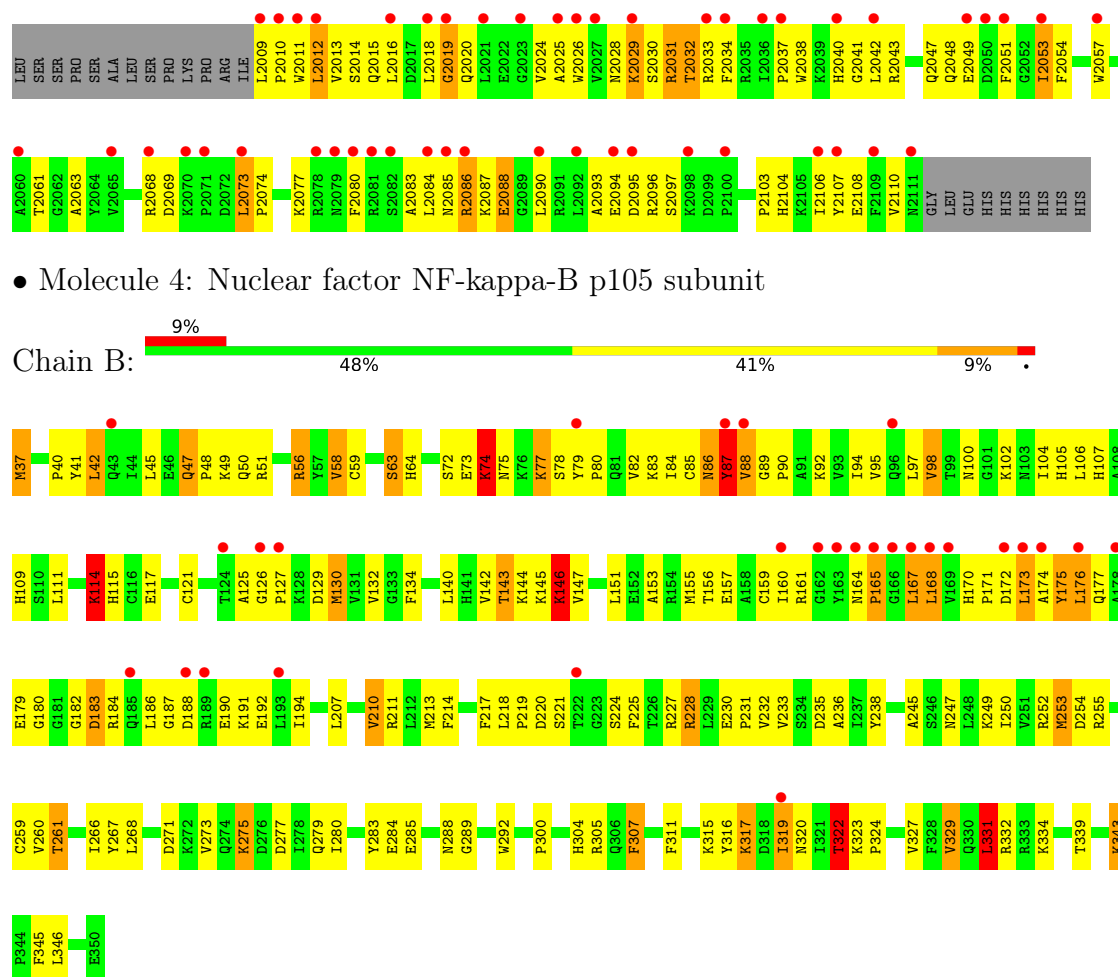
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	6	Total 6	O 6	0	0
5	F	4	Total 4	O 4	0	0
5	A	10	Total 10	O 10	0	0
5	B	5	Total 5	O 5	0	0

- Molecule 1: 36-MER



C2	A3	G4	A5	G6	G7	A8	A9	T10	T11	T12	C13	C17	T18	T19	A22	C23	T24	T25	C26	T27	C28	C29	C30	T31	T32	T33	C34	A35
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E1054	E1055	R1058	W1063	R1067	G1068	R1069	W1070	F1071	P1072	S1073	S1074	R1075	G1076	G1077	G1078	G1079	A1080	A1081	A1082	A1083	E1084	T1085	A1086	E1087	R1088	A1089	T1093	L1099	T1102	R1103	R1104	L1108	R1109	D1110	M1111	S1112	G1113	D1114	P1115	H1119	K1120	G1126	S1127	L1128	S1129	S1130	D1131	S1132	REF																																																																																																																																																																																																																																																																																																																																																																																																																					
L272	R273	R274	R275	S276	D277	R278	S281	M284	E285	F286	P290	D291	G292	S293	L294	L295	S296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L7



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.22Å 116.37Å 134.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.65 – 2.80 40.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.65-2.80) 99.8 (40.65-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.278 0.253 , 0.294	Depositor DCC
R_{free} test set	1903 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7912	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	E	0.33	0/845	0.79	1/1306 (0.1%)
2	F	0.32	0/755	0.79	0/1160
3	A	0.49	1/4094 (0.0%)	1.02	13/5547 (0.2%)
4	B	0.47	0/2524	1.02	15/3407 (0.4%)
All	All	0.46	1/8218 (0.0%)	0.98	29/11420 (0.3%)

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	E	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1012	VAL	CA-CB	6.00	1.60	1.53

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	80	ASP	CA-C-N	9.72	130.40	120.38
3	A	80	ASP	C-N-CA	9.72	130.40	120.38
3	A	81	PRO	CA-C-N	-8.27	109.51	119.84
3	A	81	PRO	C-N-CA	-8.27	109.51	119.84
3	A	81	PRO	N-CA-C	7.97	120.42	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	35	DG	C1'

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	E	750	0	407	48	0
2	F	678	0	388	60	0
3	A	3988	0	3878	231	0
4	B	2471	0	2468	185	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
5	E	6	0	0	0	0
5	F	4	0	0	0	0
All	All	7912	0	7141	505	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 34.

The worst 5 of 505 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:B:47:GLN:HG3	4:B:48:PRO:HD2	1.29	1.10
3:A:2009:LEU:HG	3:A:2087:LYS:HE3	1.32	1.09
2:F:30:DC:H2''	2:F:31:DT:H5''	1.33	1.08
3:A:2086:ARG:CG	3:A:2086:ARG:HH11	1.67	1.07
3:A:2029:LYS:H	3:A:2029:LYS:HD3	1.20	1.06

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	
3	A	490/540 (91%)	399 (81%)	60 (12%)	31 (6%)	1	3
4	B	312/314 (99%)	264 (85%)	37 (12%)	11 (4%)	3	10
All	All	802/854 (94%)	663 (83%)	97 (12%)	42 (5%)	1	5

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	81	PRO
3	A	169	SER
3	A	191	THR
3	A	1074	SER
3	A	1128	LEU

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	
3	A	423/463 (91%)	386 (91%)	37 (9%)	9	30
4	B	269/269 (100%)	238 (88%)	31 (12%)	5	18
All	All	692/732 (94%)	624 (90%)	68 (10%)	7	25

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	176	LEU
4	B	210	VAL
4	B	322	THR
3	A	1054	GLU
3	A	1037	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	279	GLN
4	B	288	ASN
3	A	263	GLN
3	A	200	ASN
4	B	304	HIS

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 oligosaccharides 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	E	36/36 (100%)	0.51	4 (11%) 10 7	30, 51, 124, 142	0
2	F	34/34 (100%)	0.31	2 (5%) 28 21	27, 48, 71, 123	0
3	A	498/540 (92%)	0.82	76 (15%) 5 4	27, 60, 122, 139	0
4	B	314/314 (100%)	0.69	28 (8%) 15 11	28, 63, 116, 140	0
All	All	882/924 (95%)	0.74	110 (12%) 8 6	27, 60, 121, 142	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	1132	SER	9.2
3	A	2012	LEU	6.4
3	A	2016	LEU	6.1
3	A	2027	VAL	5.5
3	A	2034	PHE	4.9

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 oligosaccharides 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.