



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 01:03 PM UTC

PDB ID : 1I6V / pdb_00001i6v
Title : THERMUS AQUATICUS CORE RNA POLYMERASE-RIFAMPICIN COMPLEX
Authors : Campbell, E.A.; Korzheva, N.; Mustaev, A.; Murakami, K.; Goldfarb, A.; Darst, S.A.
Deposited on : 2001-03-05
Resolution : 3.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

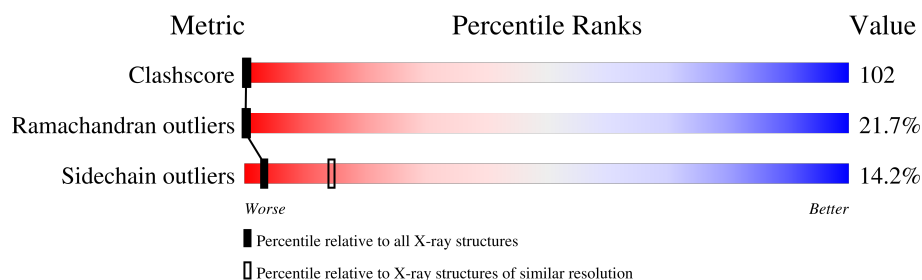
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	11% 39% 16% 5% 29%
1	B	314	10% 44% 18% • 27%
2	C	1118	11% 56% 29% •
3	D	1264	15% 49% 25% • 7%
4	E	99	17% 58% 23% ••

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21292 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 DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1741	1109	299	330	3			
1	B	230	Total	C	N	O	S	0	0	0
			1761	1122	299	337	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	VAL	GLY	conflict	UNP Q9KWU8
A	232	SER	LEU	conflict	UNP Q9KWU8
B	112	VAL	GLY	conflict	UNP Q9KWU8
B	232	SER	LEU	conflict	UNP Q9KWU8

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	conflict	UNP Q9KWU7
C	?	-	GLU	deletion	UNP Q9KWU7
C	1111	VAL	ILE	conflict	UNP Q9KWU7

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1174	Total	C	N	O	S	17	0	0
			8502	5329	1550	1596	27			

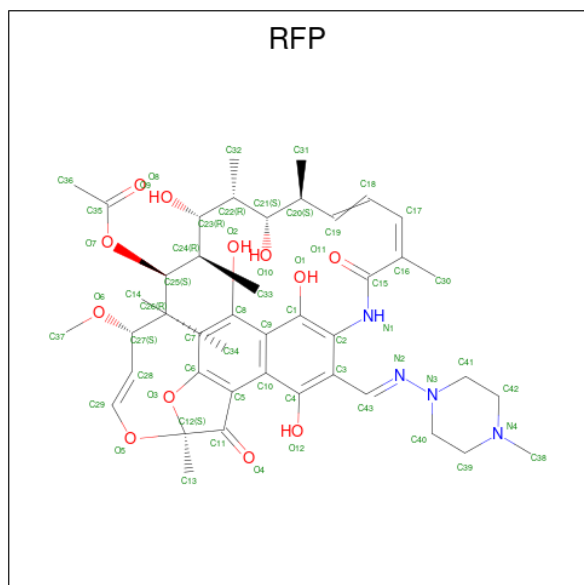
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	ALA	GLY	conflict	UNP Q9KWU6
D	77	ALA	GLY	conflict	UNP Q9KWU6
D	91	ALA	GLY	conflict	UNP Q9KWU6
D	113	ALA	GLY	conflict	UNP Q9KWU6
D	139	ALA	GLY	conflict	UNP Q9KWU6
D	144	ALA	GLY	conflict	UNP Q9KWU6
D	863	THR	VAL	conflict	UNP Q9KWU6
D	866	THR	VAL	conflict	UNP Q9KWU6
D	1009	ASN	LYS	conflict	UNP Q9KWU6

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	98	Total	C	N	O	S	0	0	0
			719	453	132	130	4			

- Molecule 5 is RIFAMPICIN (CCD ID: RFP) (formula: C₄₃H₅₈N₄O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total 1	Mg 1	0	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

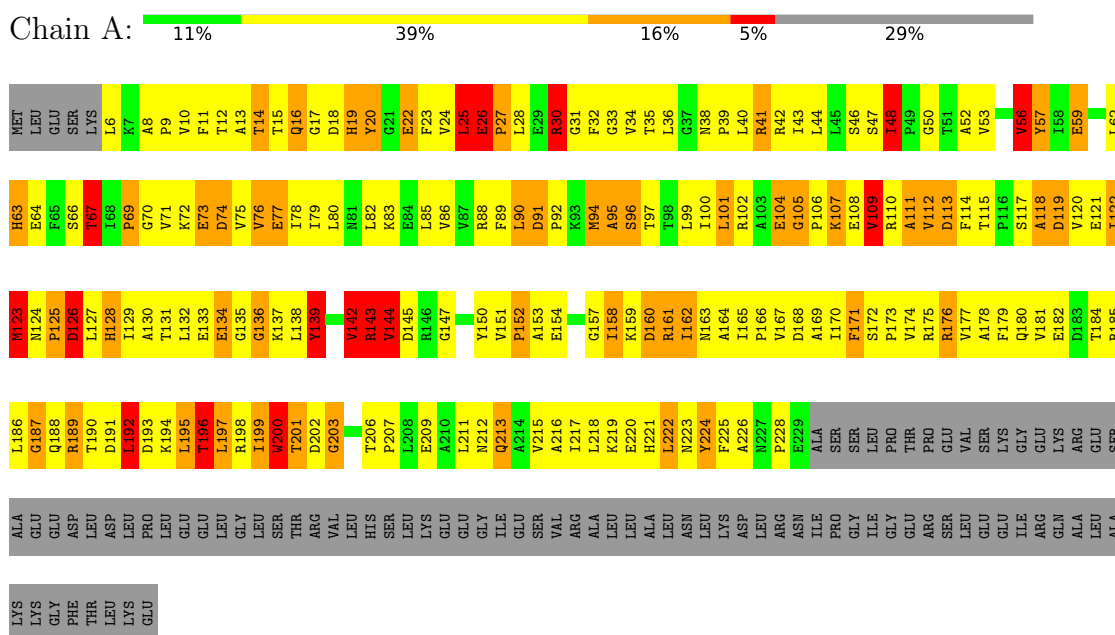
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Zn 1	0	0

3 Residue-property plots

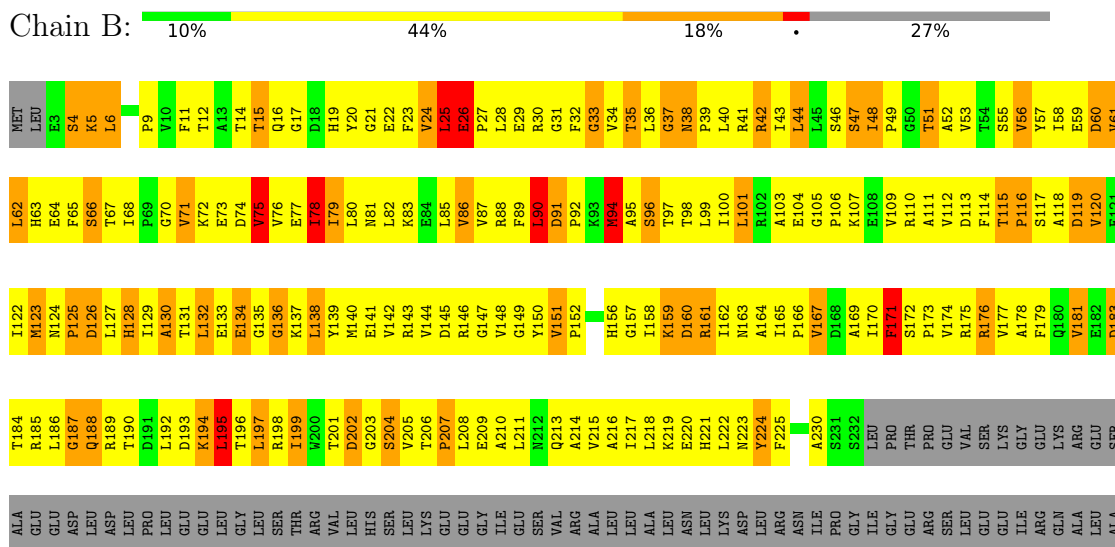
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE



• Molecule 1: DNA-DIRECTED RNA POLYMERASE



LYS
LYS
GLY
PHE
THR
LEU
LYS
GLU

● Molecule 2: DNA-DIRECTED RNA POLYMERASE

Chain C: 11% 56% 29%

E856	E796	A732	N671	T609	F549	T487	V427	L367	T306	P244	T183	M121	K61	MET	
D657	G797	A733	V672	R610	L550	A488	R428	T368	R308	G245	M184	L307	G62		
M858	G798	L734	R611	L734	E551	S489	D429	P369	L307	D246	M185	E123	G63		
P859	R735	A612	R612	A612	H552	E490	V430	A370	P309	P247	V186	G124	L64		
H860	V800	D736	A674	V613	D553	E491	H431	K371	L310	P248	N187	G125	V65		
L861	V801	L737	V676	R614	D554	D492	R432	L372	F311	K249	S126	S126	L66		
P862	R802	D738	M677	V615	E555	A493	T433	V373	A312	K250	K190	F127	D67		
D663	R803	F678	M678	V616	N556	V494	H434	F374	N318	D251	F191	N128	F68		
H864	E739	D617	F679	D617	R557	T495	V435	S375	T314	K252	P192	N129	L69		
R805	T742	L742	D680	G618	A558	T496	G436	R376	E70	A253	P193	N130	E70		
L806	V743	R619	G681	R619	L559	A497	R437	P377	G316	L254	V194	G131	V71		
R807	R744	L620	G682	L620	M560	Q498	L438	L378	V317	A255	V195		R72		
D808	R683	V621	G683	V621	G561	A499	C439	E379	P318	V256	L196		R73		
G809	G746	H623	G684	H623	S562	N500	P440	A380	G319	L257	G197	V135	G74		
L870	D810	A747	G685	P624	V563	T501	V441	A381	H320	F258	R198	N136	D75		
P811	R811	E748	D686	L625	M564	P502	E442	L382	H321	G259	V199	V137	P76		
L872	H812	V749	A687	R626	G565	L503	T443	R383	E322	L260	P177	S138	P77		
R873	V813	K750	L688	R627	T566		P444	E384	D323	L261	L200	Q139	F78		
E814			V689	V628	Q567	R507	E445	F385	D324	A262	G201	Q139	F78		
R875	L815	D753	L690	R629	A568	L508	E446	F386	L325	D263	Y202	N140	T19		
V876	K316	L754	S691	R630	V569	A509	L447	R387	X382	L269	D203	H141	Q80		
R877	P817	L755	L755	R631	T570	T510	N448	R388	D326	P264	Q204	R142	D81		
G878	V756	D761	G693	N632	L571	D511	T449	S389	L328	R266	E205	S143	Q22		
R879	G757	L694	L694	Q633	L572	R512	G450	Q390	G329	E267	L207	G145	R84		
M880	R820	R758	L695	R634	R573	V513	L451	L391	N330	D268	L208	V146	E85		
N881	E821	T759	G696	T635	A574	V514	L452	S392	R331	L269	R209	Y147	X86		
L882	V822	S760	G697	A636	Q575	A515	T453	Q393	R332	G270	E210	F148	D87		
G883	R823	F761	D698	P637	A576	R516	S454	F394	L333		L211	T149	L88		
R824	K762	R762	F699	D638	P577	R517	L455	K395	R334	G273	S212	P150	T89		
L885	V825	G763	Y700	Q1639	V578	R518	A456	D396	T335	R274	A213	D151	Y90		
R886	R826		T701	R640	V579	G519	A457	E397	V336		Y214	P152	Q91		
E887	V827		S702	P641	M580	E520	V458	T398	G337	K276	G214	A153	A92		
L888	R768	L703	L703	R642	T581	P521	L464	R405	F344	G283	L221	N159	X38		
G829	P769	H704	V643	V643	G582	V522	G465	L404	R340	G284	L222	Q160	Q99		
R889	R829	R705	R644	R644	L583	L523	F466	K407	V346	L285	D223	S161	X40		
L890	E770	L706	L705	V645	L584	L524	D462	K407	V346	S286	E224	I162	N41		
R831	R771	R706	R706	V645	E584	V524	D462	K407	V346	G287	A225	I163	V42		
K832	R772		R707	G646	E585	A525	A463	S403	A341	L281	Q219	R157	P36		
L833	L773			G647	E586	P526	L464	F405	D342	G282	G220	R158	E37		
Q834	L774			R648	V587	R527	G465	R405	F344	G283	L221	Q160	X38		
V835	R775		T710		V588	E528	F466	K407	V346	L285	D223	S161	X40		
R836	R776		V711		V588	V529	D467	K407	V346	S286	E224	I162	N41		
R896	S776		R712		R589	V529	D467	K407	V346	G287	A225	I163	V42		
L897	I777		R713		D590	E530	R468	R408	G347				H102		
G838	R778		D714		S591	F531	T469	R409	L348	R288	V226	P164	K103		
R839	G779		T715		L592	M532	P470	T410	A349	T289	L104	L165	D104		
R900	A840		K716		E593	D533	V471	A411	R350	L290	A228	P166	T105		
N901	N841		R717		A594	V534	R472	A412	R351	G291	M229	K167	Q45		
L902	R842		G718		L595	S535	R473	L413	A352	R292	R330	R168	G106		
S903	H843		G719		V596	P536	R474	L414	A352	R292	R330	R168	L107		
G944	G844		F720		E597	K537	V474	G414	R353	F293	G169	K108	F48		
N905	N845		R721		E598	P537	R475	G415	R354	E294	K109	P170	X49		
V906	K846		T722		Q538	V539	N476	G416	V355	D295	E232	V171	E50		
D907	G847		R723		E599	Q539	R477	G417	R356	G296	A234	N172	D111		
V848	V788		R724		D600	F540	V478	L418	E357	E297	M235	D173	F52		
A908	R849		R725		G601	S541	R479	T419	R358	F298	V236	L174	P53		
					E602	L542	T480	R420	M559	K299	R237	E175	F114		
T910	A850		T726		V603	N543	E481	R421	V360	D300	E176	K115	L115		
E911	R851		T727		V604	T544	E482	R422	M361	E301	E177	K117	G57		
P912	L852		H728		K605	N545	V483	R423	G362	D301	E177	K117	D58		
E913	L853		R793		V606	L546	V484	R424	S363	F303	G180	G180	P58		
	P854		S730		D607	L547	V485	R425	G364	R304	L241	X181	G57		
T914	R855		R731		E608	D547	V486	F426	P364	L305	R242	V181	P119		

- Molecule 4: DNA-DIRECTED RNA POLYMERASE

[illegible]

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	199.45Å 199.45Å 289.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.276 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21292	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, RFP

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	0.56	0/1775	1.11	12/2417 (0.5%)
1	B	0.59	1/1795 (0.1%)	1.16	13/2447 (0.5%)
2	C	0.54	0/8672	1.21	107/11752 (0.9%)
3	D	0.60	2/8439 (0.0%)	1.30	123/11447 (1.1%)
4	E	0.47	0/730	1.15	7/991 (0.7%)
All	All	0.57	3/21411 (0.0%)	1.23	262/29054 (0.9%)

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	0	1
2	C	0	1
3	D	0	3
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	ALA	C-N	-19.61	1.06	1.33
1	B	94	MET	SD-CE	12.20	2.10	1.79
3	D	1268	PRO	C-N	5.74	1.41	1.33

The worst 5 of 262 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	O-C-N	-22.83	92.23	122.59
3	D	1270	ALA	CA-C-N	17.97	155.87	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	C-N-CA	17.97	155.87	121.54
3	D	775	GLY	N-CA-C	17.26	127.55	111.67
3	D	834	THR	N-CA-C	-14.30	95.86	114.31

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
2	C	1013	TYR	Sidechain
3	D	1165	TYR	Sidechain
3	D	1268	PRO	Mainchain
3	D	1270	ALA	Mainchain

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	1741	0	1747	367	0
1	B	1761	0	1754	336	0
2	C	8508	0	8421	1917	0
3	D	8502	0	8002	1758	0
4	E	719	0	685	142	0
5	C	59	0	56	6	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
All	All	21292	0	20665	4262	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 102.

The worst 5 of 4262 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)
1:B:94:MET:CE	1:B:94:MET:SD	2.10	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:690:ILE:HB	2:C:852:ILE:HG22	1.19	1.18
2:C:565:GLN:HG3	2:C:995:MET:HE1	1.25	1.16
3:D:1280:VAL:HG12	3:D:1281:VAL:HG23	1.25	1.16
2:C:491:GLU:HA	2:C:531:PHE:HA	1.29	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	222/314 (71%)	111 (50%)	61 (28%)	50 (22%)	0	0
1	B	228/314 (73%)	123 (54%)	62 (27%)	43 (19%)	0	0
2	C	1111/1118 (99%)	591 (53%)	277 (25%)	243 (22%)	0	0
3	D	1126/1264 (89%)	588 (52%)	291 (26%)	247 (22%)	0	0
4	E	96/99 (97%)	50 (52%)	24 (25%)	22 (23%)	0	0
All	All	2783/3109 (90%)	1463 (53%)	715 (26%)	605 (22%)	0	0

5 of 605 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	19	HIS
1	A	26	GLU
1	A	59	GLU
1	A	73	GLU

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	189/271 (70%)	159 (84%)	30 (16%)	2	12
1	B	190/271 (70%)	166 (87%)	24 (13%)	4	18
2	C	870/935 (93%)	754 (87%)	116 (13%)	4	17
3	D	782/1035 (76%)	661 (84%)	121 (16%)	2	12
4	E	67/88 (76%)	60 (90%)	7 (10%)	7	25
All	All	2098/2600 (81%)	1800 (86%)	298 (14%)	3	14

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1038	LEU
3	D	1447	LEU
3	D	1061	PHE
3	D	1190	SER
2	C	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1333	HIS
3	D	1374	GLN
2	C	1639	GLN
2	C	632	ASN
3	D	1393	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	RFP	C	1640	-	63,63,63	1.28	8 (12%)	94,94,94	0.96	4 (4%)

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
5	RFP	C	1640	-	-	15/60/85/85	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1640	RFP	O5-C29	3.51	1.48	1.39
5	C	1640	RFP	O4-C11	3.37	1.27	1.21
5	C	1640	RFP	C5-C10	3.14	1.49	1.42
5	C	1640	RFP	C8-C9	2.99	1.51	1.43
5	C	1640	RFP	C39-N4	2.66	1.52	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1640	RFP	C5-C10-C9	-2.60	115.41	119.77
5	C	1640	RFP	C34-C26-C25	-2.41	107.15	111.40
5	C	1640	RFP	C24-C23-C22	2.14	118.97	115.41
5	C	1640	RFP	O12-C4-C10	2.08	124.19	119.17

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

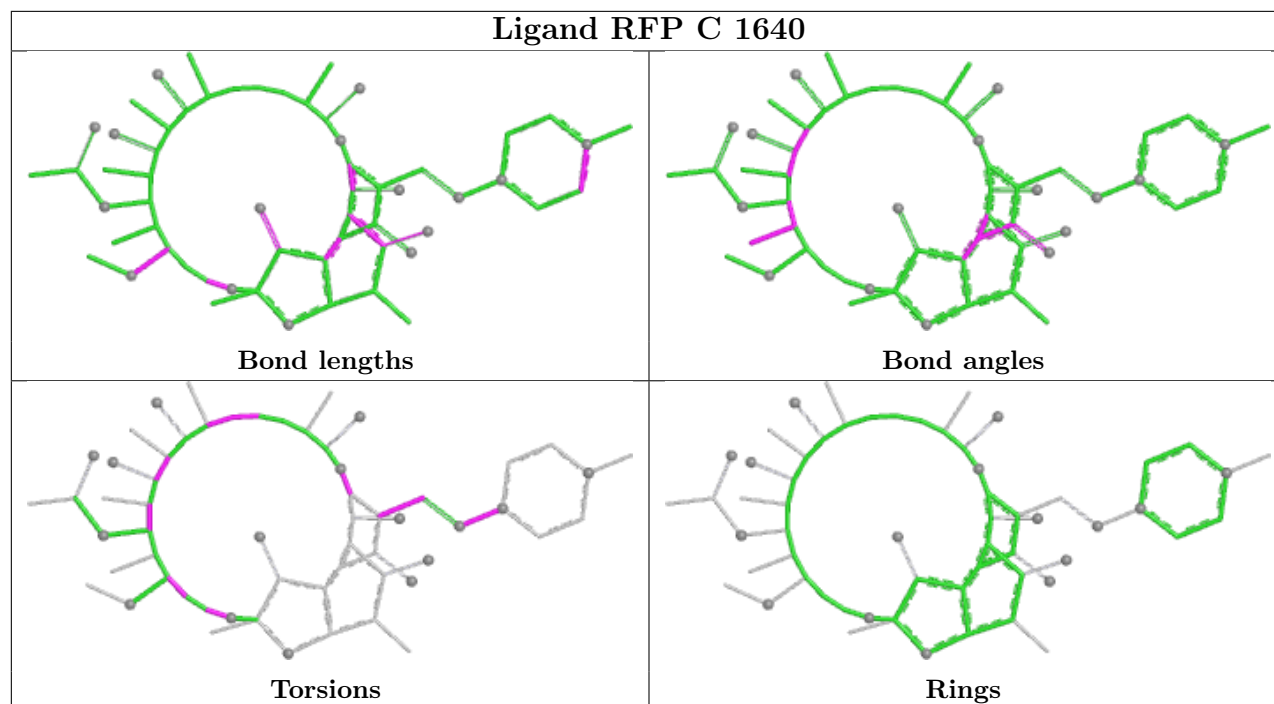
Mol	Chain	Res	Type	Atoms
5	C	1640	RFP	C17-C18-C19-C20
5	C	1640	RFP	C26-C27-C28-C29
5	C	1640	RFP	O6-C27-C28-C29
5	C	1640	RFP	C32-C22-C23-C24
5	C	1640	RFP	C21-C22-C23-C24

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1640	RFP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	155:ASP	C	2(U):UNK	N	54.72
1	D	46(U):UNK	C	452:ILE	N	47.08
1	D	10(U):UNK	C	20(U):UNK	N	15.58
1	D	1270:ALA	C	1271:LYS	N	1.06

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.