



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:59 PM GMT

PDB ID : 1I6V
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
<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

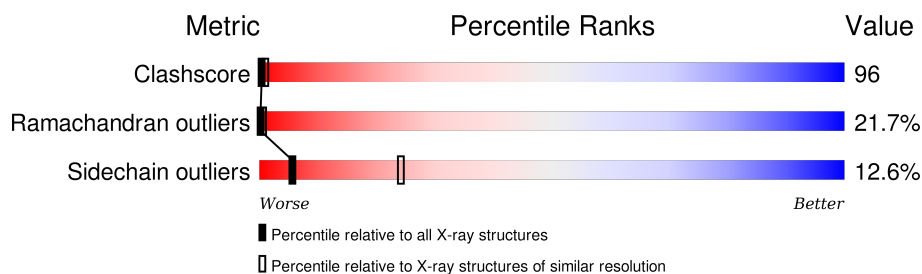
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
2	C	1118	
3	D	1264	
4	E	99	

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			

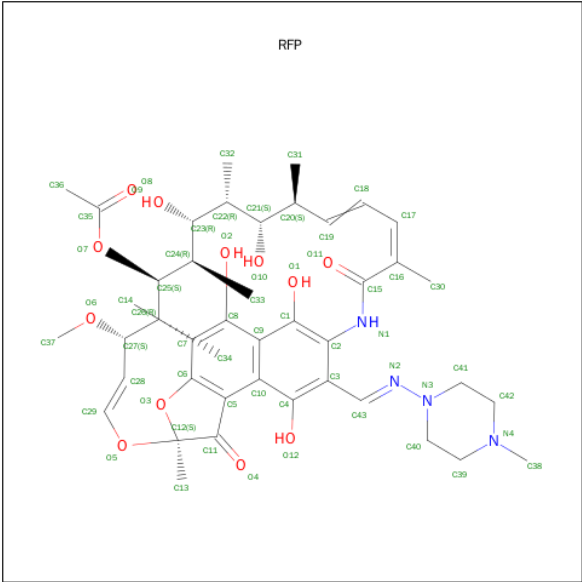
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is RIFAMPICIN (three-letter code: RFP) (formula: C₄₃H₅₈N₄O₁₂).



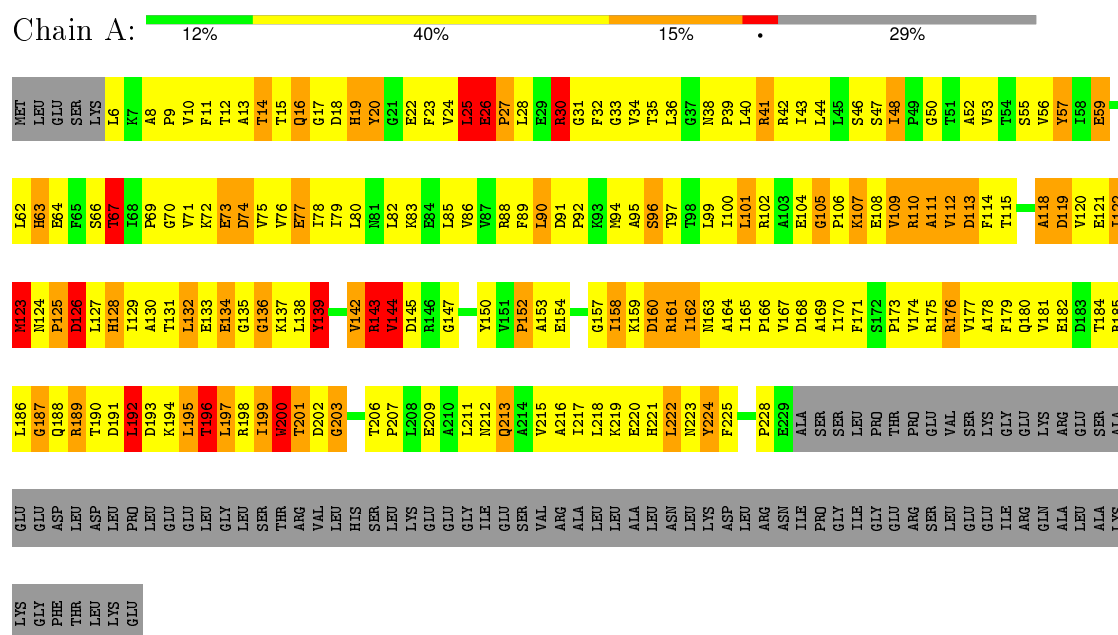
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			59	43	4	12		

3 Residue-property plots

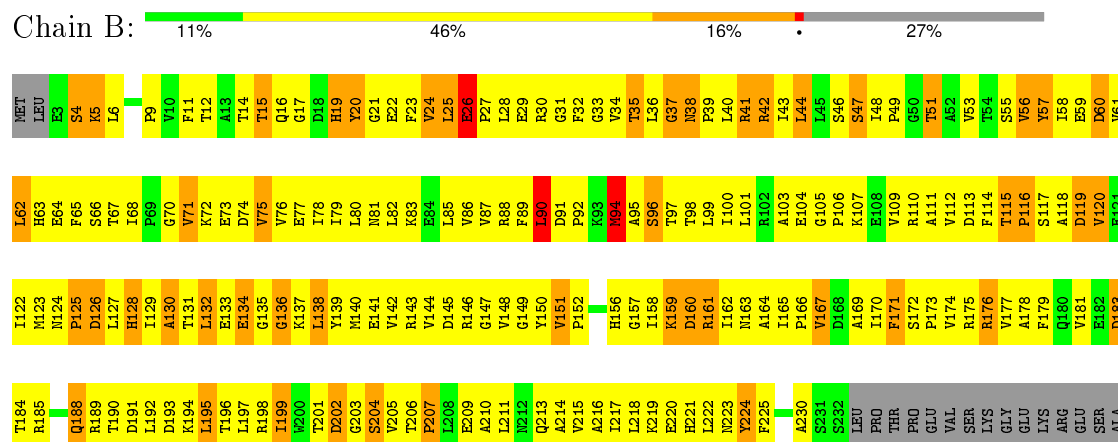
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE




• Molecule 1: DNA-DIRECTED RNA POLYMERASE



GLU	LYS
GLU	GLY
ASP	PHE
LEU	THR
ASP	LEU
LEU	LYS
PRO	LEU
LEU	GLU
GLU	GLU
LEU	LEU
GLY	LEU
LEU	GLY
SER	THR
THR	ARG
VAL	VAL
GLU	GLY
GLY	GLY
ILE	ILE
GLU	GLU
LEU	LEU
ASN	ASN
LEU	LEU
LYS	LYS
ASP	ASP
LEU	LEU
ARG	ARG
ASN	ASN
ILE	ILE
PRO	PRO
GLY	GLY
ILE	ILE
GLY	GLY
ARG	ARG
SER	SER
LEU	LEU
GLU	GLU
GLU	GLU
ILE	ILE
ARG	ARG
GLN	GLN
ALA	ALA
LEU	LEU
ALA	ALA
LYS	LYS

• Molecule 2: DNA-DIRECTED RNA POLYMERASE

Chain C:  14% 60% 24%

MET	G62	T122	M184	G246	Y309	A370	H431	E491	D553	B616	D680	I742	R805
R2	G63	E123	K185	D246	L310	K371	R432	D491	D554	D617	G681	V743	L806
I3	L64	D124	M187	P248	F311	L372	T433	R493	A555	G618	N682	R744	R807
R4	V65	G125	M187	P248	F311	N373	T434	Y494	N556	R619	N683	I745	
R5	L66	S126	K190	K250	T314	N374	Y435	T495	R557	V621	F684	G746	D810
R6	D67	S127	K191	K251	T315	N375	R436	I496	A558	H623	E685	A747	P811
G7	F68	I128	F191	D251	A315	R376	R437	A497	L559	H624	D686	E748	G812
R8	L69	I129	F192	K252	G316	F377	I438	Q498	M560	L625	A687	V749	G813
R9	E70	G131	L193	K253	P317	L378	Q439	A499	G561	L626	N688	K750	E814
R10	Y71		L194	L254	G318	A380	P440	N500	M564	R626	V689	D753	L815
E11	Y72		L195	A255	P319	E379	P441	T501	Q565	R627	G690	I754	K816
Y12	I73		L196	A256	G320	A381	V442	P502	T566	Y628	S691	P754	P817
I13	G74		L197	L257	E321	L382	T443	L503	Q567	A629	E692	L755	G818
P14	D75		R198	F268	V322	R383	P444	R507	A568	R630	E693	V756	V819
L15	P76		V199	G259	D323	E384	E445	R508	A569	S631	L694	G757	R820
P16	P77		L200	L260	D324	F385	G446	L508	F568	N632	L695	E758	R821
P17	F78		G201	L261	R331	Q392	A447	A509	A570	Q633	R696	T759	V822
Y18	S79		Y202	A262	R332	Q393	N448	T510	P571	G634	R697	T760	V823
L19	Q80		D203	D263	H327	R388	I449	D511	L571	G635	D698	F761	R824
E20	D81		Q204	P264	L328	L391	G450	R512	A572	A636	F699	K762	V825
I21	L88		E205	K265	T335	L451	L451	R513	A573	P637	Y700	G763	R826
Q22	C83		T206	R266	R330	Q392	I452	V514	Q575	V643	E706	E764	A828
Y23	R84		L207	T267	R331	Q393	T453	A515	A576	R640	T707		
E24	E85		V208	D268	R332	F394	S454	R516	P577	R641	I703	S768	R831
S25	K86		R209	L269	R333	K395	L455	R517	Q578	R642	H704	E769	K832
Y26	D87		E210	G270	R334	D396	A456	R518	V579	V643	I705	E770	L833
R27	L88		L211		T335	E397	A457	G519	M580	R644	E706	R771	R834
K28	L89		S212		V336	T398	Y458	E520	F587	R645	T707	R772	Q834
A29	Y90		A213		R337	Q399	A459	P521	G582	V645	L710	L773	V835
L30	Q91		Y214		E338	P400	R460	V522	L583	G646	I711	L774	G836
A92	A92		D215		L339	L401	V461	I523	E584	Q647	E712	R775	D837
A32	P93		D216		N340	S402	D462	V524	E585	R648	A712	S776	K838
D33	L94		L217		A341	S403	A463	A525	R586		R713	I777	L839
V34	Y95		V218		D342	L404	L464	P526	F587	D653	R714	F778	A840
P35	A96		Q219		Q343	R405	G465	E527	V588	L654	T715	G779	N841
R97	R97		G220		F344	H406	F466	E528	R589	L655	K716	E780	R842
E37	L98		L221		R345	K407	I467	V529		A656	L717	K781	H843
K38	Q99		L222		V346	R408	R468	E530	L592	D657	G718	A782	G844
R39	L100		D223		G347	R409	T469	P531	L595	G658	F719	R783	N845
V42	I101		E224		L348	L410	P470	N532	L596	P659	E720	D784	K846
G43	H102		A225		A349	S411	Y471	D533	Y596	A660	R721	K785	G847
Q43	K103		V226		R350	A412	R472	V534	A597	S661	I722	K786	V848
I44	D104		L227		L351	G413	R473	S535	E598	E662	R723	D787	V849
Q45	T105		A228		A352	L414	V474	P536	E599	B663	R724	T788	A850
A46	G106		M229		R353	P415	K475	K537	D600	G664	D725	S789	K851
A47	L107		R230		G354	G416	N476	Q538	G601	F665	I726	L790	L852
R49	K108		P231		V355	G417	G477	V539	E602	L666	P727	R791	G847
E50	K109		E232		R356	L418	V478	P540	V603	A667	H728	V792	L853
E51	E110		E233		E357	T419	V479	S541	V604	L668	R729	P793	V854
T51	D111		A234		R358	R420	T480	L542	K605	G669	S730	P794	V855
F52	E112		R235		M359	E421	E481	N543	V606	Q670	E731	G795	D856
P53	V113		V236		V360	R422	E482	T544	D607	N671	A732	E796	N857
I54	F114		R237		M361	A423	V483	N545	G608	V672	A733	E797	N858
E55	L115		L238		G362	G424	V484	L546	T609	L673	H734	G798	P859
E56	G116		P239		S363	F425	Y485	P547	R610	V674	T735	V799	H860
G57	H117		T240		P364	D426	V486	P548	L611	A675	R736	V800	P861
B58	L118		L241		F305	V427	T487	P549	A612	L676	L737	R801	D863
R59	P119		R242		T306	R428	A488	E551	V613	P677	H738	G802	G864
G60	L120		R243		L307	D429	S489	R550	R614	P678	E739	R803	T865
M61	M121		P244		R308	V430	E490	H552	V615	F679	L804		P866



V1466	I1467	I1468	G1469	R1470	L1471	I1472	P1473	A1474	G1475	T1476	G1477	S1478	D1479	F1480	V1481	R1482	F1483	T1484	Q1485	V1486	V1487	D1488	Q1489	R1490	T1491	L1492	E1496	GIU	ALA	ARG	GLU	LYS	GLY	ALA	ALA	VAL	VAL	GLU	LYS	LYS	GLU	PRO	ARG	ARG	ARG	GLU	GLN	PRO	GLY	GLY	GLY
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	--------------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	--------------	-------	--------------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain E: 19% 62% 18%

M63	M64	M65	M66	M67	M68	M69	M70	M71	M72	M73	M74	M75	M76	M77	M78	M79	M80	M81	M82	M83	M84	M85	M86	M87	M88	M89	M90	M91	M92	M93	M94	M95	M96	M97	M98	M99	M100	M101	M102	M103	M104	M105	M106	M107	M108	M109	M110	M111	M112	M113	M114	M115	M116	M117	M118	M119	M120	M121	M122	M123	M124	M125	M126	M127	M128	M129	M130	M131	M132	M133	M134	M135	M136	M137	M138	M139	M140	M141	M142	M143	M144	M145	M146	M147	M148	M149	M150	M151	M152	M153	M154	M155	M156	M157	M158	M159	M160	M161	M162	M163	M164	M165	M166	M167	M168	M169	M170	M171	M172	M173	M174	M175	M176	M177	M178	M179	M180	M181	M182	M183	M184	M185	M186	M187	M188	M189	M190	M191	M192	M193	M194	M195	M196	M197	M198	M199	M200	M201	M202	M203	M204	M205	M206	M207	M208	M209	M210	M211	M212	M213	M214	M215	M216	M217	M218	M219	M220	M221	M222	M223	M224	M225	M226	M227	M228	M229	M230	M231	M232	M233	M234	M235	M236	M237	M238	M239	M240	M241	M242	M243	M244	M245	M246	M247	M248	M249	M250	M251	M252	M253	M254	M255	M256	M257	M258	M259	M260	M261	M262	M263	M264	M265	M266	M267	M268	M269	M270	M271	M272	M273	M274	M275	M276	M277	M278	M279	M280	M281	M282	M283	M284	M285	M286	M287	M288	M289	M290	M291	M292	M293	M294	M295	M296	M297	M298	M299	M300	M301	M302	M303	M304	M305	M306	M307	M308	M309	M310	M311	M312	M313	M314	M315	M316	M317	M318	M319	M320	M321	M322	M323	M324	M325	M326	M327	M328	M329	M330	M331	M332	M333	M334	M335	M336	M337	M338	M339	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353	M354	M355	M356	M357	M358	M359	M360	M361	M362	M363	M364	M365	M366	M367	M368	M369	M370	M371	M372	M373	M374	M375	M376	M377	M378	M379	M380	M381	M382	M383	M384	M385	M386	M387	M388	M389	M390	M391	M392	M393	M394	M395	M396	M397	M398	M399	M400	M401	M402	M403	M404	M405	M406	M407	M408	M409	M410	M411	M412	M413	M414	M415	M416	M417	M418	M419	M420	M421	M422	M423	M424	M425	M426	M427	M428	M429	M430	M431	M432	M433	M434	M435	M436	M437	M438	M439	M440	M441	M442	M443	M444	M445	M446	M447	M448	M449	M450	M451	M452	M453	M454	M455	M456	M457	M458	M459	M460	M461	M462	M463	M464	M465	M466	M467	M468	M469	M470	M471	M472	M473	M474	M475	M476	M477	M478	M479	M480	M481	M482	M483	M484	M485	M486	M487	M488	M489	M490	M491	M492	M493	M494	M495	M496	M497	M498	M499	M500	M501	M502	M503	M504	M505	M506	M507	M508	M509	M510	M511	M512	M513	M514	M515	M516	M517	M518	M519	M520	M521	M522	M523	M524	M525	M526	M527	M528	M529	M530	M531	M532	M533	M534	M535	M536	M537	M538	M539	M540	M541	M542	M543	M544	M545	M546	M547	M548	M549	M550	M551	M552	M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571	M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590	M591	M592	M593	M594	M595	M596	M597	M598	M599	M600	M601	M602	M603	M604	M605	M606	M607	M608	M609	M610	M611	M612	M613	M614	M615	M616	M617	M618	M619	M620	M621	M622	M623	M624	M625	M626	M627	M628	M629	M630	M631	M632	M633	M634	M635	M636	M637	M638	M639	M640	M641	M642	M643	M644	M645	M646	M647	M648	M649	M650	M651	M652	M653	M654	M655	M656	M657	M658	M659	M660	M661	M662	M663	M664	M665	M666	M667	M668	M669	M670	M671	M672	M673	M674	M675	M676	M677	M678	M679	M680	M681	M682	M683	M684	M685	M686	M687	M688	M689	M690	M691	M692	M693	M694	M695	M696	M697	M698	M699	M700	M701	M702	M703	M704	M705	M706	M707	M708	M709	M710	M711	M712	M713	M714	M715	M716	M717	M718	M719	M720	M721	M722	M723	M724	M725	M726	M727	M728	M729	M730	M731	M732	M733	M734	M735	M736	M737	M738	M739	M740	M741	M742	M743	M744	M745	M746	M747	M748	M749	M750	M751	M752	M753	M754	M755	M756	M757	M758	M759	M760	M761	M762	M763	M764	M765	M766	M767	M768	M769	M770	M771	M772	M773	M774	M775	M776	M777	M778	M779	M780	M781	M782	M783	M784	M785	M786	M787	M788	M789	M790	M791	M792	M793	M794	M795	M796	M797	M798	M799	M800	M801	M802	M803	M804	M805	M806	M807	M808	M809	M810	M811	M812	M813	M814	M815	M816	M817	M818	M819	M820	M821	M822	M823	M824	M825	M826	M827	M828	M829	M830	M831	M832	M833	M834	M835	M836	M837	M838	M839	M840	M841	M842	M843	M844	M845	M846	M847	M848	M849	M850	M851	M852	M853	M854	M855	M856	M857	M858	M859	M860	M861	M862	M863	M864	M865	M866	M867	M868	M869	M870	M871	M872	M873	M874	M875	M876	M877	M878	M879	M880	M881	M882	M883	M884	M885	M886	M887	M888	M889	M890	M891	M892	M893	M894	M895	M896	M897	M898	M899	M900	M901	M902	M903	M904	M905	M906	M907	M908	M909	M910	M911	M912	M913	M914	M915	M916	M917	M918	M919	M920	M921	M922	M923	M924	M925	M926	M927	M928	M929	M930	M931	M932	M933	M934	M935	M936	M937	M938	M939	M940	M941	M942	M943	M944	M945	M946	M947	M948	M949	M950	M951	M952	M953	M954	M955	M956	M957	M958	M959	M960	M961	M962	M963	M964	M965	M966	M967	M968	M969	M970	M971	M972	M973	M974	M975	M976	M977	M978	M979	M980	M981	M982	M983	M984	M985	M986	M987	M988	M989	M990	M991	M992	M993	M994	M995	M996	M997	M998	M999	M1000	M1001	M1002	M1003	M1004	M1005	M1006	M1007	M1008	M1009	M1010	M1011	M1012	M1013	M1014	M1015	M1016	M1017	M1018	M1019	M1020	M1021	M1022	M1023	M1024	M1025	M1026	M1027	M1028	M1029	M1030	M1031	M1032	M1033	M1034	M1035	M1036	M1037	M1038	M1039	M1040	M1041	M1042	M1043	M1044	M1045	M1046	M1047	M1048	M1049	M1050	M1051	M1052	M1053	M1054	M1055	M1056	M1057	M1058	M1059	M1060	M1061	M1062	M1063	M1064	M1065	M1066	M1067	M1068	M1069	M1070	M1071	M1072	M1073	M1074	M1075	M1076	M1077	M1078	M1079	M1080	M1081	M1082	M1083	M1084	M1085	M1086	M1087	M1088	M1089	M1090	M1091	M1092	M1093	M1094	M1095	M1096	M1097	M1098	M1099	M1100	M1101	M1102	M1103	M1104	M1105	M1106	M1107	M1108	M1109	M1110	M1111	M1112	M1113	M1114	M1115	M1116	M1117	M1118	M1119	M1120	M1121	M1122	M1123	M1124	M1125	M1126	M1127	M1128	M1129	M1130	M1131	M1132	M1133	M1134	M1135	M1136	M1137	M1138	M1139	M1140	M1141	M1142	M1143	M1144	M1145	M1146	M1147	M1148	M1149	M1150	M1151	M1152	M1153	M1154	M1155	M1156	M1157	M1158	M1159	M1160	M1161	M1162	M1163	M1164	M1165	M1166	M1167	M1168	M1169	M1170	M1171	M1172	M1173	M1174	M1175	M1176	M1177	M1178	M1179	M1180	M1181	M1182	M1183	M1184	M1185	M1186	M1187	M1188	M1189	M1190	M1191	M1192	M1193	M1194	M1195	M1196	M1197	M1198	M1199	M1200	M1201	M1202	M1203	M1204	M1205	M1206	M1207	M1208	M1209	M1210	M1211	M1212	M1213	M1214	M1215	M1216	M1217	M1218	M1219	M1220	M1221	M1222	M1223	M1224	M1225	M1226	M1227	M1228	M1229	M1230	M1231	M1232	M1233	M1234	M1235	M1236	M1237	M1238	M1239	M1240	M1241	M1242	M1243	M1244	M1245	M1246	M1247	M1248	M1249	M1250	M1251	M1252	M1253	M1254	M1255	M1256	M1257	M1258	M1259	M1260	M1261	M1262	M1263	M1264	M1265	M1266	M1267	M1268	M1269	M1270	M1271	M1272	M1273	M1274	M1275	M1276	M1277	M1278	M1279	M1280	M1281	M1282	M1283	M1284	M1285	M1286	M1287	M1288	M1289	M1290	M1291	M1292	M1293	M1294	M1295	M1296	M1297	M1298	M1299	M1300	M1301	M1302	M1303	M1304	M1305	M1306	M1307	M1308	M1309	M1310	M1311	M1312	M1313	M1314	M1315	M1316	M1317	M1318	M1319	M1320	M1321	M1322	M1323	M1324	M1325	M1326	M1327	M1328	M1329	M1330	M1331	M1332	M1333	M1334	M1335	M1336	M1337	M1338	M1339	M1340	M1341	M1342	M1343	M1344	M1345	M1346	M1347	M1348	M1349	M1350	M1351	M1352	M1353	M1354	M1355	M1356	M1357	M1358	M1359	M1360	M1361	M1362	M1363	M1364	M1365	M1366	M1367	M1368	M1369	M1370	M1371	M1372	M1373	M1374	M1375	M1376	M1377	M1378	M1379	M1380	M1381	M1382	M1383	M1384	M1385	M1386	M1387	M1388	M1389	M1390	M1391	M1392	M1393	M1394	M1395	M1396	M1397	M1398	M1399	M1400	M1401	M1402	M1403	M1404	M1405	M1406	M1407	M1408	M1409	M1410	M1411	M1412	M1413	M1414	M1415	M1416	M1417	M1418	M1419	M1420	M1421	M1422	M1423	M1424	M1425	M1426	M1427	M1428	M1429	M1430	M1431	M1432	M1433	M1434	M1435	M1436	M1437	M1438	M1439	M1440	M1441	M1442	M1443	M1444	M1445	M1446	M1447	M1448	M1449	M1450	M1451	M1452	M1453	M1454	M1455	M1456	M1457	M1458	M1459	M1460	M1461	M1462	M1463	M1464	M1465	M1466	M1467	M1468	M1469	M1470	M1471	M1472	M1473	M1474	M1475	M1476	M1477	M1478	M1479	M1480	M1481	M1482	M1483	M1484	M1485	M1486	M1487	M1488	M1489	M1490	M1491	M1492	M1493	M1494	M1495	M1496	M1497	M1498	M1499	M1500	M1501	M1502	M1503	M1504	M1505	M1506	M1507	M1508	M1509	M1510	M1511	M1512	M1513	M1514	M1515	M1516	M1517	M1518	M1519	M1520	M1521	M1522	M1523	M1524	M1525	M1526	M1527	M1528	M1529	M1530	M1531	M1532	M1533	M1534	M1535	M1536	M1537	M1538	M1539	M1540	M1541	M1542	M1543	M1544	M1545	M1546</
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	---------

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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, RFP, MG

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	0.43	0/1775	0.77	1/2417 (0.0%)
1	B	0.42	1/1795 (0.1%)	0.77	1/2447 (0.0%)
2	C	0.41	0/8672	0.80	7/11752 (0.1%)
3	D	0.44	1/8439 (0.0%)	0.84	19/11447 (0.2%)
4	E	0.37	0/730	0.71	0/991
All	All	0.42	2/21411 (0.0%)	0.81	28/29054 (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	0	1
2	C	0	1
3	D	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	ALA	C-N	-12.09	1.06	1.34
1	B	94	MET	SD-CE	5.75	2.10	1.77

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	O-C-N	-19.05	92.23	122.70
3	D	1270	ALA	C-N-CA	13.67	155.87	121.70
3	D	1270	ALA	CA-C-N	12.08	143.77	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	580	MET	N-CA-C	6.98	129.85	111.00
3	D	1166	LEU	CA-CB-CG	6.22	129.61	115.30

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	348	0
1	B	1761	0	1754	316	0
2	C	8508	0	8421	1817	0
3	D	8502	0	8002	1671	0
4	E	719	0	685	138	0
5	D	1	0	0	0	0
6	D	1	0	0	0	0
7	C	59	0	56	6	0
All	All	21292	0	20665	4041	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 96.

The worst 5 of 4041 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:SD	1:B:94:MET:CE	2.10	1.39
2:C:690:ILE:HB	2:C:852:ILE:HG22	1.19	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:772:PRO:HG3	3:D:778:LEU:HB2	1.28	1.14

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	1
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%)	161 (85%)	28 (15%)	4	17
1	B	190/271 (70%)	169 (89%)	21 (11%)	8	31
2	C	870/935 (93%)	770 (88%)	100 (12%)	7	29
3	D	782/1035 (76%)	671 (86%)	111 (14%)	4	19
4	E	67/88 (76%)	62 (92%)	5 (8%)	17	52
All	All	2098/2600 (81%)	1833 (87%)	265 (13%)	5	24

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	710	ILE
2	C	1115	LEU
3	D	1299	PHE
2	C	743	VAL
2	C	859	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	872	ASN
2	C	1030	GLN
3	D	1374	GLN
2	C	881	ASN
2	C	962	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
7	RFP	C	1640	-	63,63,63	1.12	6 (9%)	82,94,94	1.02	6 (7%)

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
7	RFP	C	1640	-	-	0/60/85/85	0/1/5/5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1640	RFP	C42-N4	2.17	1.51	1.46
7	C	1640	RFP	C8-C9	2.46	1.51	1.43
7	C	1640	RFP	C5-C10	2.48	1.49	1.43
7	C	1640	RFP	O4-C11	2.64	1.27	1.21
7	C	1640	RFP	C39-N4	2.91	1.52	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1640	RFP	C34-C26-C25	-2.26	107.15	111.38
7	C	1640	RFP	C5-C10-C9	-2.03	115.41	119.73
7	C	1640	RFP	C20-C21-C22	2.01	117.54	114.24
7	C	1640	RFP	C24-C23-C22	2.29	118.97	115.25
7	C	1640	RFP	C2-N1-C15	2.41	128.65	123.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

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

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.