



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 03:54 AM EDT

PDB ID : 5EXR / pdb_00005exr
Title : Crystal structure of human primosome
Authors : Tahirov, T.H.; Baranovskiy, A.G.; Babayeva, N.D.
Deposited on : 2015-11-24
Resolution : 3.60 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:

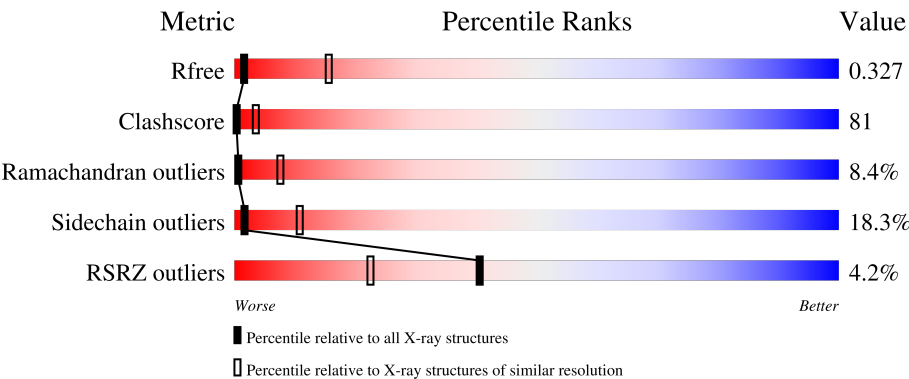
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	A	420	21% 18%60%15%7%
1	E	420	6% 21%60%11%7%
2	B	509	3% 17%44%21%15%
2	F	509	5% 15%44%23%15%
3	C	1128	% 18%51%22%6%

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Mol	Chain	Length	Quality of chain
3	G	1128	
4	D	597	
4	H	597	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SF4	B	601	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37658 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 primase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3261	2099	564	583	15			
1	E	389	Total	C	N	O	S	0	0	0
			3261	2099	564	583	15			

- Molecule 2 is a protein called DNA primase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	434	Total	C	N	O	S	0	0	0
			3562	2280	616	653	13			
2	F	434	Total	C	N	O	S	0	0	0
			3562	2280	616	653	13			

- Molecule 3 is a protein called DNA polymerase alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1057	Total	C	N	O	S	0	0	0
			8544	5477	1433	1578	56			
3	G	1057	Total	C	N	O	S	0	0	0
			8544	5477	1433	1578	56			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	ALA	VAL	engineered mutation	UNP P09884
G	516	ALA	VAL	engineered mutation	UNP P09884

- Molecule 4 is a protein called DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	444	Total	C	N	O	S	0	0	0
			3451	2194	576	666	15			

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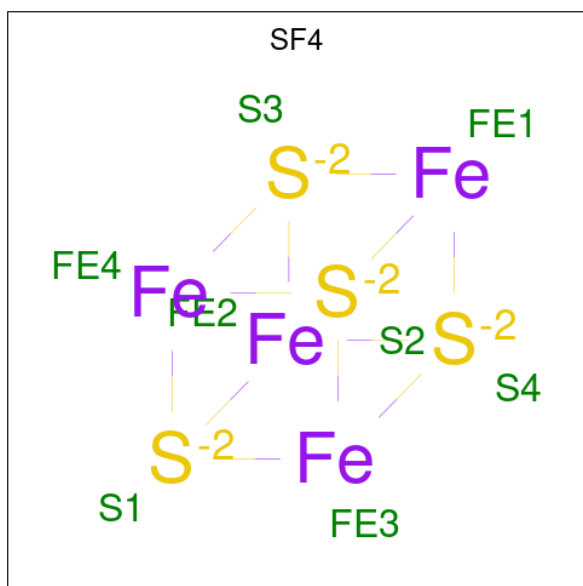
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	444	Total	C	N	O	S	0	0	0
			3451	2194	576	666	15			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	C	2	Total	Zn	0	0
			2	2		
5	E	1	Total	Zn	0	0
			1	1		
5	G	2	Total	Zn	0	0
			2	2		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

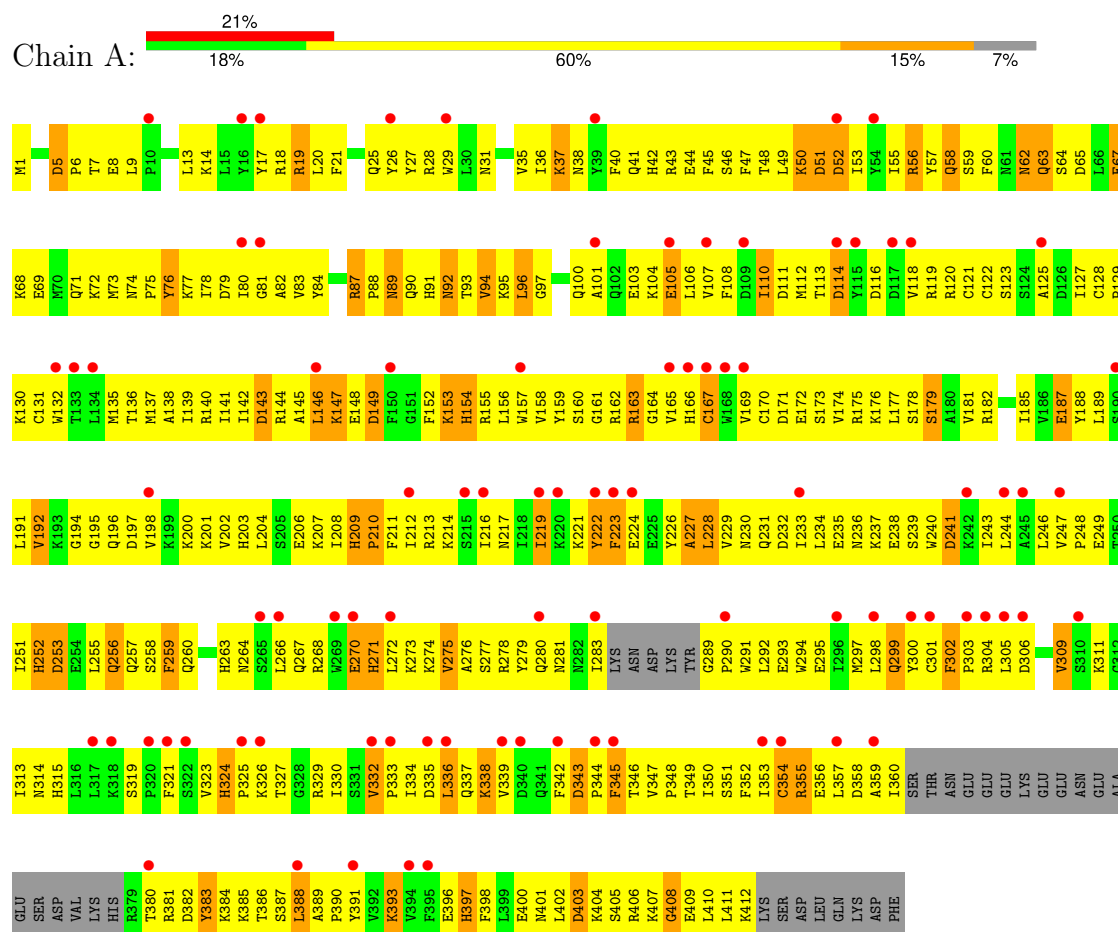


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	F	1	Total	Fe	S	0	0
			8	4	4		

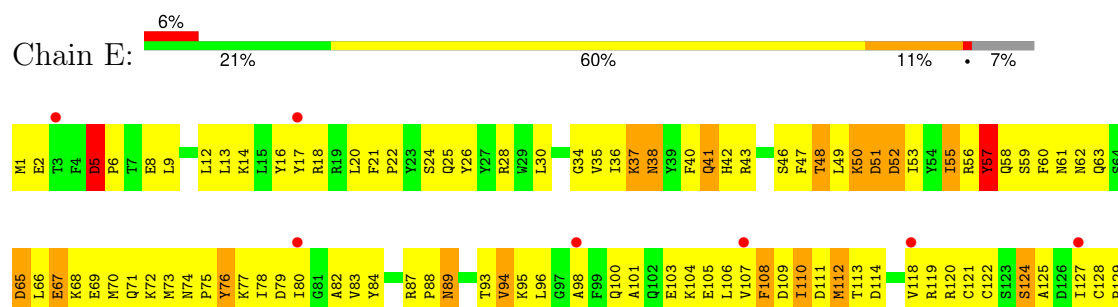
3 Residue-property plots [i](#)

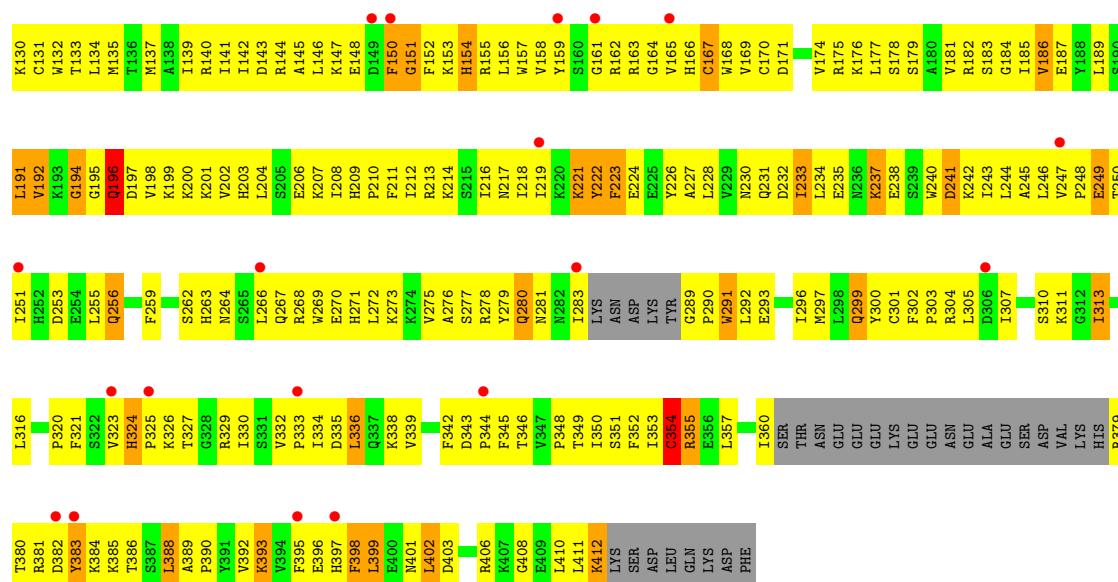
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA primase small subunit

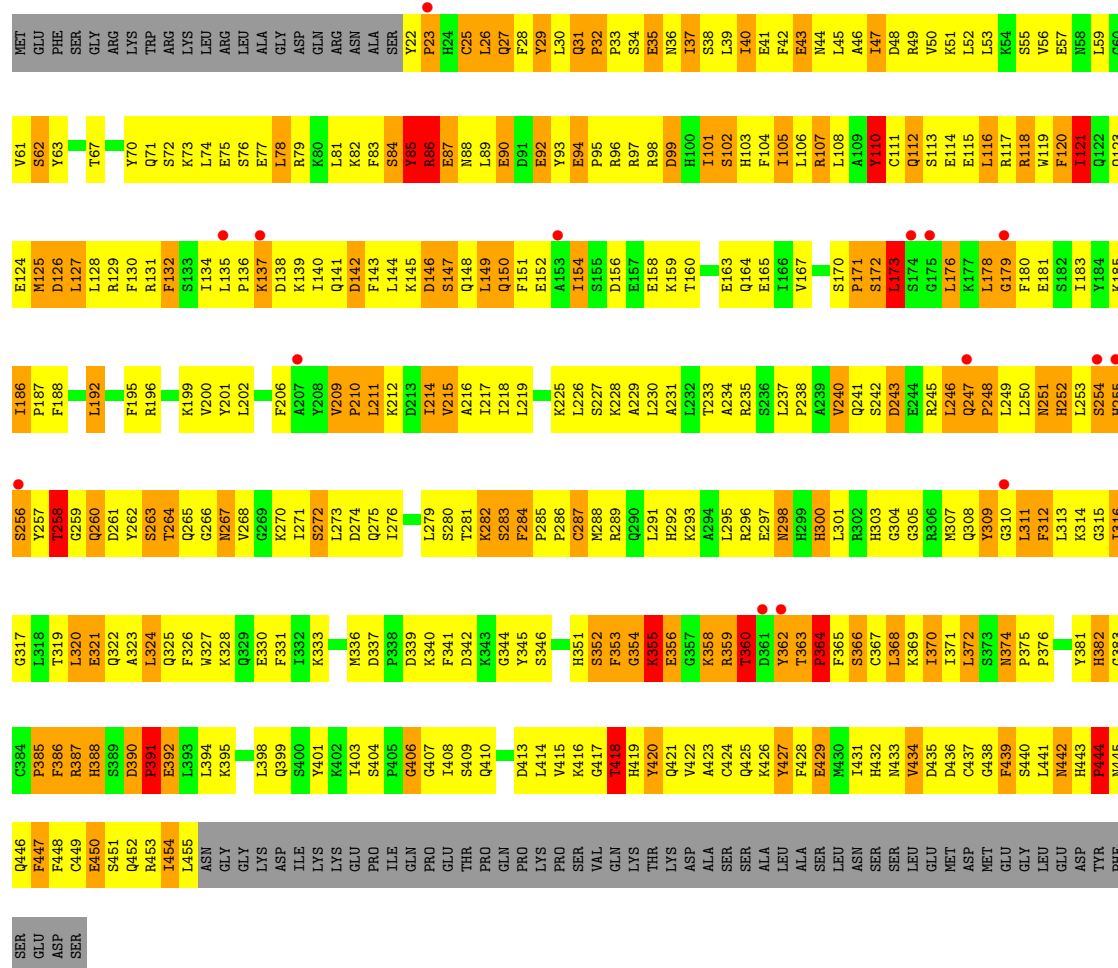
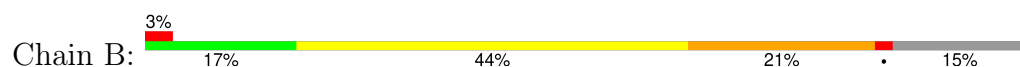


• Molecule 1: DNA primase small subunit

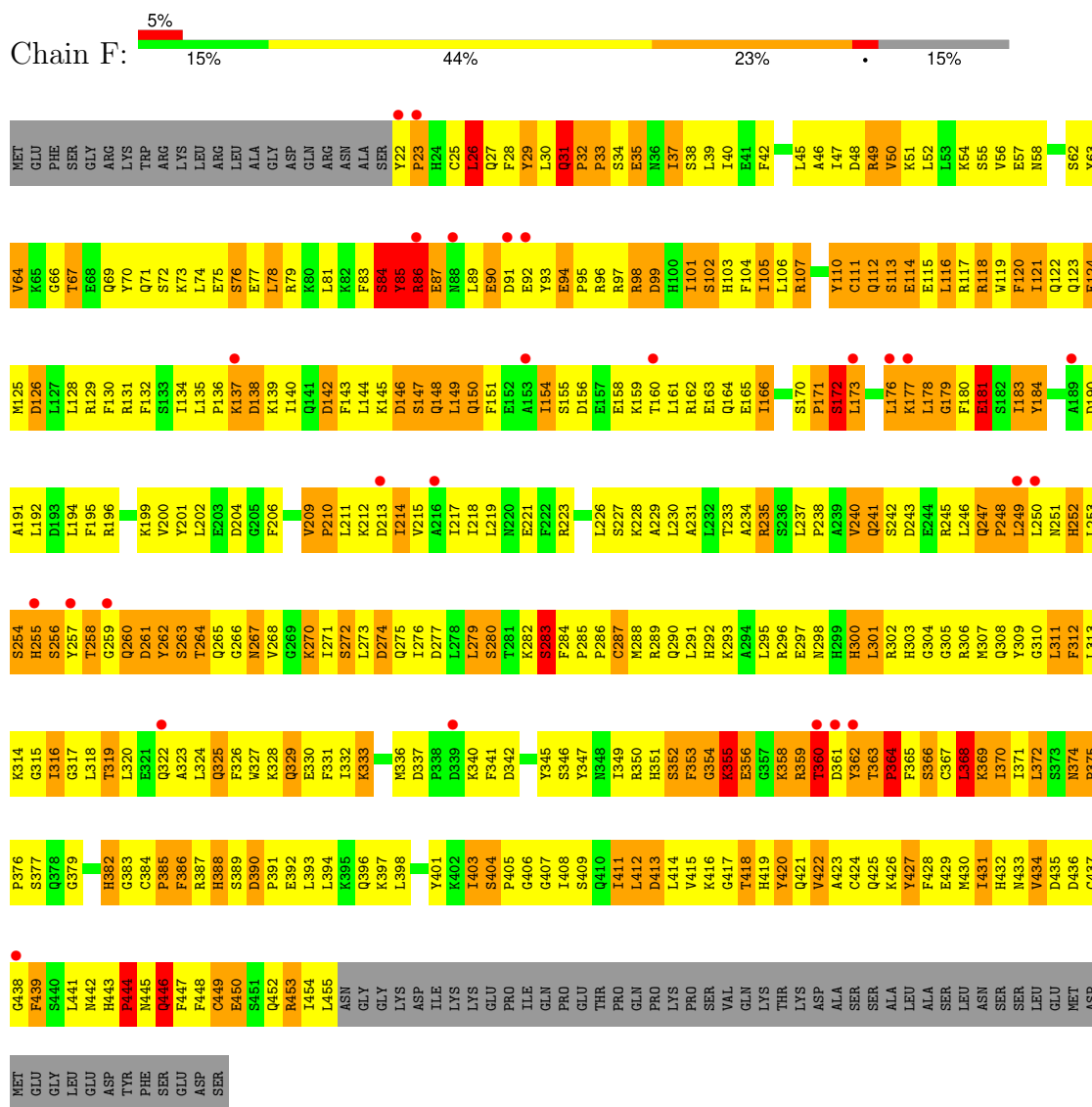




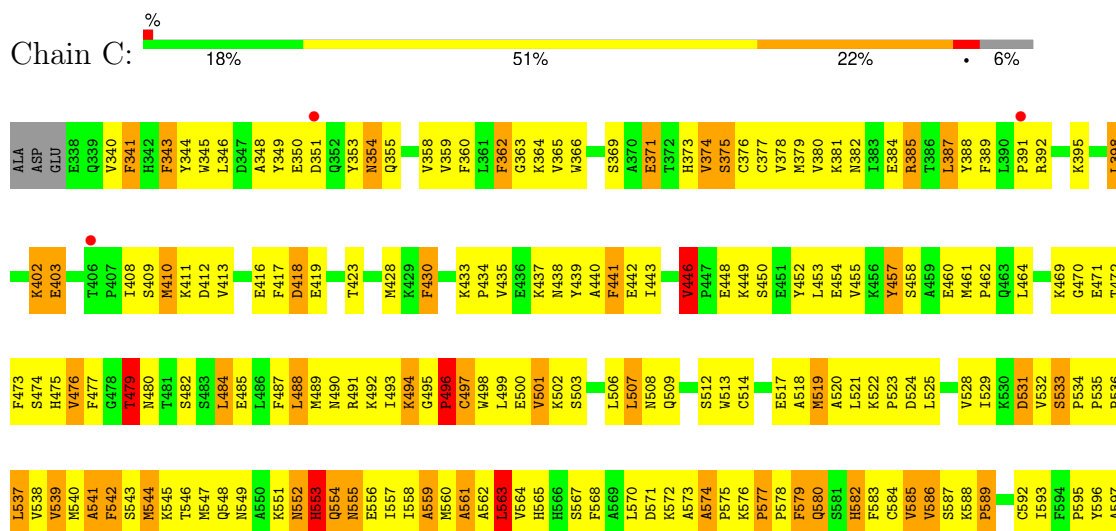
• Molecule 2: DNA primase large subunit



• Molecule 2: DNA primase large subunit



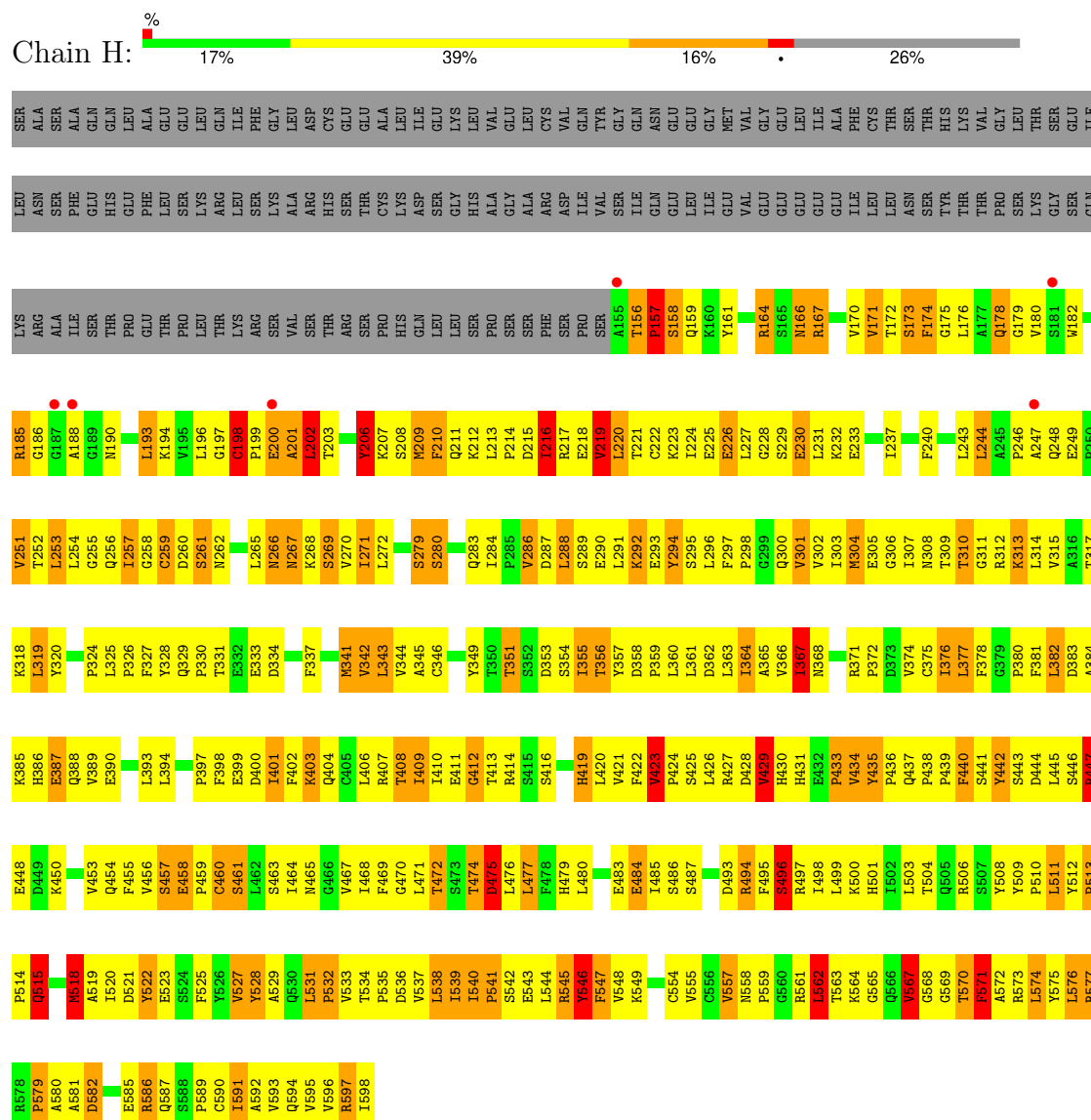
• Molecule 3: DNA polymerase alpha catalytic subunit



L1405	Y1341	Q1214	K1150	D1090	N1023	F962	P902	G842	W721	H658	F598
E1406	Y1342	Q1215	S1151	T1091	K1024	S965	D903	L843	W722	W659	K599
K1407	E1277	I1216	P1152	G1092	V1025	S966	P904	W844	T723	S660	E600
L1408	R1278	L1217	P1153	N1093	K1026	R966	S905	L845	F724	K661	V601
T1409	F1279	F1218	H1154	F1094	S1027	F967	L906	D846	W725	I662	I602
T1410	L1346	V1219	V1155	V1095	E1028	V968	E907	P847	W726	G663	E603
D1411	C1281	V1220	H1156	L1096	V1029	A969	N908	K848	W727	K664	K604
H1412	F1282	A1221	V1157	G1097	N1030	K970	G909	W849	W728	L665	K605
E1413	C1283	R1222	A1158	Q1098	K1031	P971	I910	G850	W729	K666	K606
E1414	L1283	I1223	L1159	I1099	L1032	L972	I911	F851	W730	L667	V607
D1415	P1351	C1224	W1160	A973	L1100	A973	P912	Y852	W731	L792	K608
K1416	T1352	E1289	L1161	S1101	K1034	A974	R913	L793	W732	R913	V609
L1417	C1353	P1226	N1162	D1102	L1035	L975	E914	K854	W733	P671	E610
K1418	R1354	I1227	S1163	Q1103	L1038	V976	I915	F855	W734	K672	V611
K1419	N1355	I1230	R1167	E1105	E1037	T977	R916	L856	E735	LEU	A612
Q1420	Y1292	D1231	R1168	R1105	I1038	T978	K917	L857	W736	GLY	A613
F1421	T1357	A1232	F1168	T1107	D1039	K979	L918	L858	W737	GLY	T614
F1422	N1295	E1233	V1169	T1107	L1040	G980	V919	L859	W738	ARG	E615
T1423	F1296	V1233	K1170	I1108	D1041	R981	E920	D860	W739	SER	R616
K1424	L1360	L1234	A1171	V1109	G1042	E982	R921	F861	W740	GLY	T617
K1425	G1300	I1235	V1175	E1110	V1043	I983	R922	N862	L741	PHE	L618
V1426	T1301	A1236	S1176	N1111	F1044	L984	K923	S863	L742	G680	L619
L1427	D1302	T1237	V1177	I1112	K1045	N985	Q924	L864	E743	G620	F621
Q1428	M1303	W1238	Y1178	Q1113	S1046	H986	V925	W865	H744	R682	F622
D1429	E1304	L1239	V1179	K1114	L1047	T987	K926	P866	T745	K683	L623
Y1430	P1305	G1240	I1179	R1115	L1048	K988	Q927	S867	W746	G687	A624
K1431	S1306	L1241	C1180	L1116	L1049	E989	L928	L868	D747	R688	K625
K1432	L1307	P1242	Q1181	I1117	L1050	N990	M929	L869	D748	R689	V626
L1433	C1371	P1243	D1182	E1118	K1051	V991	K930	Q870	A749	M690	K627
K1434	P1372	T1244	G1183	I1119	L1058	E997	P936	F876	K750	L690	K628
N1435	C1310	Q1245	S1184	G1120	K1054	K993	Q932	F872	F751	C691	I629
T1436	S1311	F1246	H1185	E1121	Y1055	H994	D933	N873	I752	D692	I629
A1437	L1437	R1247	L1186	N1122	A1056	N995	L934	L874	L753	V693	D630
E1438	L1313	V1248	T1187	V1123	A1057	L996	C875	E694	Q754	E694	P631
Q1439	D1314	H1249	A1188	L1124	L1058	E997	P936	F876	W755	L695	P632
F1440	T1378	H1250	S1189	N1125	L1063	V998	D937	W877	C757	S696	I633
L1441	L1379	Y1251	Q1190	G1126	S1064	I999	L938	W878	ASP	A697	I634
S1442	Q1380	H1252	R1191	S1127	D1065	Y1000	I939	W879	GLU	K698	V635
R1443	P1381	K1253	A1192	V1128	D1066	G1001	Q941	Q880	ASP	E699	G636
S1444	E1382	D1254	Y1193	P1129	N1067	T1002	L940	R881	GLU	L700	H637
G1445	Y1383	E1255	A1194	V1130	N1067	T1003	D943	W882	ILE	R702	N638
Y1446	S1384	E1256	P1195	S1131	Y1068	D1004	D943	ALA	L762	R702	I639
S1447	D1385	N1257	E1196	Q1132	L1068	S1005	I944	SER	F763	C703	V640
E1448	K1386	D1258	Q1197	F1133	E1073	I1006	E945	GLU	L764	K704	G641
V1449	S1387	ALA	L1198	E1134	L1074	M1007	Q946	ALA	A765	ASP	F642
N1450	L1388	LEU	Q1199	I1135	K1075	I1008	K947	GLN	L766	THR	E643
L1451	Y1389	LEU	K1200	N1136	G1076	N1009	A948	LYS	Q767	H706	L644
L1452	T1390	GLY	Q1201	K1137	L1077	T1010	L949	VAL	I768	L708	E645
L1453	K1329	GLY	D1202	A1138	D1078	N1011	K950	THR	T769	S709	V646
F1454	Q1391	PRO	N1203	L1139	T1079	S1012	L951	GLU	W770	E710	L647
L1455	L1392	ALA	L1204	T1140	V1080	T1013	T952	ASP	I771	L711	L648
A1456	C1393	ALA	T1205	K1141	R1081	N1014	A953	GLY	A772	L712	Q649
GLY	F1394	Q1266	I1206	D1142	R1082	L1015	N954	GLU	G773	ARG	R650
CYS	Y1395	L1267	T1207	P1143	D1083	E1016	S955	GLN	W774	LYS	I651
ALA	R1396	T1268	D1207	Q1144	W1084	E1017	N956	GLU	T775	LYS	N652
VAL	Y1397	D1269	T1208	Q1145	G1085	L1018	Y957	GLN	W776	L716	V653
LYS	L1398	E1270	Q1209	Y1145	D1086	F1019	G958	GLN	S777	K717	C654
LYS	F1397	E1271	Y1210	Y1146	D1087	F1019	C959	GLN	W778	T718	R655
LYS	F1399	D1272	Y1211	P1147	L1087	K1020	E900	GLN	R779	E719	A656
ALA	D1400	I1273	Y1212	P1148	A1088	L1021	L960	ALA	W780	R720	P657
ALA	A1401	R1274	A1213	K1149	K1089	G1022	G961	ALA	L780		

- Molecule 3: DNA polymerase alpha catalytic subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.10Å 210.16Å 172.56Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	39.94 – 3.60 39.94 – 3.60	Depositor EDS
% Data completeness (in resolution range)	68.9 (39.94-3.60) 79.0 (39.94-3.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.326 0.276 , 0.327	Depositor DCC
R_{free} test set	4621 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 134.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	37658	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4935e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4

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	0.59	0/3343	1.18	42/4508 (0.9%)
1	E	0.53	0/3343	1.10	27/4508 (0.6%)
2	B	0.67	0/3646	1.22	38/4908 (0.8%)
2	F	0.67	0/3646	1.21	41/4908 (0.8%)
3	C	0.69	1/8724 (0.0%)	1.25	91/11788 (0.8%)
3	G	0.69	3/8724 (0.0%)	1.25	95/11788 (0.8%)
4	D	0.73	0/3529	1.26	35/4795 (0.7%)
4	H	0.73	1/3529 (0.0%)	1.27	33/4795 (0.7%)
All	All	0.67	5/38484 (0.0%)	1.23	402/51998 (0.8%)

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
2	B	0	2
2	F	0	1
3	C	0	1
3	G	0	1
4	D	0	1
4	H	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1235	ILE	CA-CB	-5.81	1.47	1.54
3	G	538	VAL	CA-CB	-5.29	1.47	1.53
3	G	1233	VAL	CA-CB	-5.20	1.48	1.54
4	H	356	THR	CA-CB	-5.03	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	561	ALA	CA-C	-5.02	1.49	1.53

The worst 5 of 402 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	513	PRO	CA-C-N	15.72	135.48	119.76
4	H	513	PRO	C-N-CA	15.72	135.48	119.76
4	D	513	PRO	CA-C-N	15.05	134.81	119.76
4	D	513	PRO	C-N-CA	15.05	134.81	119.76
3	C	1447	SER	N-CA-C	-14.62	94.76	112.89

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	110	TYR	Sidechain
2	B	309	TYR	Sidechain
3	C	740	TYR	Sidechain
4	D	349	TYR	Sidechain
2	F	110	TYR	Sidechain

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	3261	0	3247	463	0
1	E	3261	0	3247	431	0
2	B	3562	0	3542	586	0
2	F	3562	0	3542	587	0
3	C	8544	0	8632	1512	0
3	G	8544	0	8634	1518	0
4	D	3451	0	3425	559	0
4	H	3451	0	3425	550	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	E	1	0	0	0	0
5	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	0	3	0
6	F	8	0	0	0	0
All	All	37658	0	37694	6075	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 81.

The worst 5 of 6075 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)
3:G:858:LEU:HD13	3:G:1007:MET:HG3	1.23	1.21
2:B:209:VAL:HG12	2:B:210:PRO:HD2	1.25	1.19
4:D:476:LEU:HD11	4:D:502:ILE:HD11	1.22	1.14
1:E:20:LEU:HD21	1:E:357:LEU:HD22	1.16	1.13
3:C:1279:PHE:HB2	3:C:1395:TYR:HE1	1.15	1.12

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	383/420 (91%)	326 (85%)	45 (12%)	12 (3%)	3	25
1	E	383/420 (91%)	336 (88%)	36 (9%)	11 (3%)	3	26
2	B	432/509 (85%)	291 (67%)	93 (22%)	48 (11%)	0	4
2	F	432/509 (85%)	295 (68%)	84 (19%)	53 (12%)	0	4
3	C	1047/1128 (93%)	731 (70%)	226 (22%)	90 (9%)	0	7
3	G	1047/1128 (93%)	743 (71%)	209 (20%)	95 (9%)	0	6
4	D	442/597 (74%)	325 (74%)	79 (18%)	38 (9%)	0	7
4	H	442/597 (74%)	330 (75%)	73 (16%)	39 (9%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4608/5308 (87%)	3377 (73%)	845 (18%)	386 (8%)	0	7

5 of 386 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
2	B	29	TYR
2	B	35	GLU
2	B	90	GLU
2	B	94	GLU

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	
1	A	363/393 (92%)	321 (88%)	42 (12%)	5	25
1	E	363/393 (92%)	322 (89%)	41 (11%)	5	26
2	B	394/459 (86%)	325 (82%)	69 (18%)	2	12
2	F	394/459 (86%)	316 (80%)	78 (20%)	1	8
3	C	962/1013 (95%)	773 (80%)	189 (20%)	1	8
3	G	962/1013 (95%)	774 (80%)	188 (20%)	1	9
4	D	390/526 (74%)	311 (80%)	79 (20%)	1	8
4	H	390/526 (74%)	305 (78%)	85 (22%)	1	7
All	All	4218/4782 (88%)	3447 (82%)	771 (18%)	2	11

5 of 771 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	248	PRO
3	G	806	LYS
2	F	319	THR
2	F	247	GLN
3	G	523	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	397	HIS
2	F	445	ASN
2	F	58	ASN
2	F	275	GLN
3	G	566	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](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
6	SF4	F	601	2	0,12,12	-	-	-		
6	SF4	B	601	2	0,12,12	-	-	-		

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
6	SF4	F	601	2	-	-	0/6/5/5
6	SF4	B	601	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	SF4	3	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 [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	389/420 (92%)	1.30	87 (22%) 2 2	39, 101, 121, 137	0
1	E	389/420 (92%)	0.89	26 (6%) 24 15	45, 98, 115, 136	0
2	B	434/509 (85%)	0.47	15 (3%) 47 27	5, 61, 112, 135	0
2	F	434/509 (85%)	0.53	26 (5%) 27 17	4, 64, 115, 135	0
3	C	1057/1128 (93%)	0.19	14 (1%) 75 48	1, 51, 93, 123	0
3	G	1057/1128 (93%)	0.26	17 (1%) 70 43	2, 54, 96, 116	0
4	D	444/597 (74%)	0.22	3 (0%) 84 61	1, 44, 94, 111	0
4	H	444/597 (74%)	0.26	6 (1%) 73 46	2, 47, 94, 121	0
All	All	4648/5308 (87%)	0.42	194 (4%) 40 22	1, 60, 109, 137	0

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	SER	5.0
3	C	680	GLY	4.3
1	A	296	ILE	4.3
4	H	200	GLU	4.1
3	G	850	GLY	3.9

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	E	501	1/1	0.97	0.06	91,91,91,91	0
5	ZN	A	501	1/1	0.98	0.09	123,123,123,123	0
5	ZN	G	1501	1/1	0.98	0.05	78,78,78,78	0
6	SF4	F	601	8/8	0.98	0.05	1,1,8,18	0
5	ZN	C	1502	1/1	0.99	0.03	26,26,26,26	0
6	SF4	B	601	8/8	0.99	0.04	1,1,2,9	0
5	ZN	C	1501	1/1	0.99	0.02	46,46,46,46	0
5	ZN	G	1502	1/1	1.00	0.03	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.