



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:39 PM GMT

PDB ID : 4YFK
Title : Escherichia coli RNA polymerase in complex with squaramide compound 8.
Authors : Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.;
McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

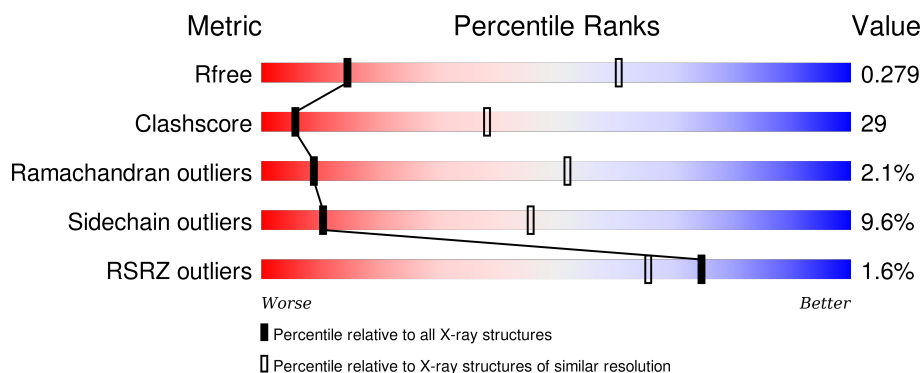
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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}	91344	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>2%</div> <div>37% 45% 14% . .</div> </div>
1	B	329	<div> <div>%</div> <div>30% 33% . 34%</div> </div>
1	G	329	<div> <div>33% 30% 6% 31%</div> </div>
1	H	329	<div> <div>2%</div> <div>28% 34% . 34%</div> </div>
2	C	1342	<div> <div>%</div> <div>48% 46% 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

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
8	4C6	D	2004	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55782 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9050	5690	1620	1694	46			
3	J	1152	Total	C	N	O	S	0	0	0
			8990	5654	1608	1682	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

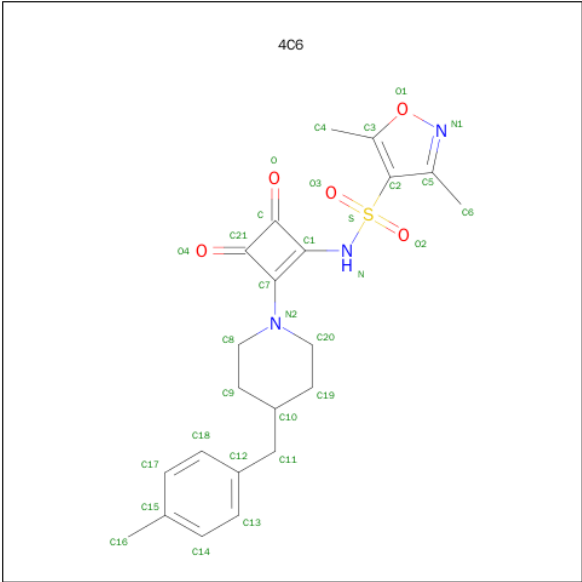
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

- Molecule 8 is 3,5-dimethyl-N-{2-[4-(4-methylbenzyl)piperidin-1-yl]-3,4-dioxocyclobut-1-en-1-yl}-1,2-oxazole-4-sulfonamide (three-letter code: 4C6) (formula: C₂₂H₂₅N₃O₅S).

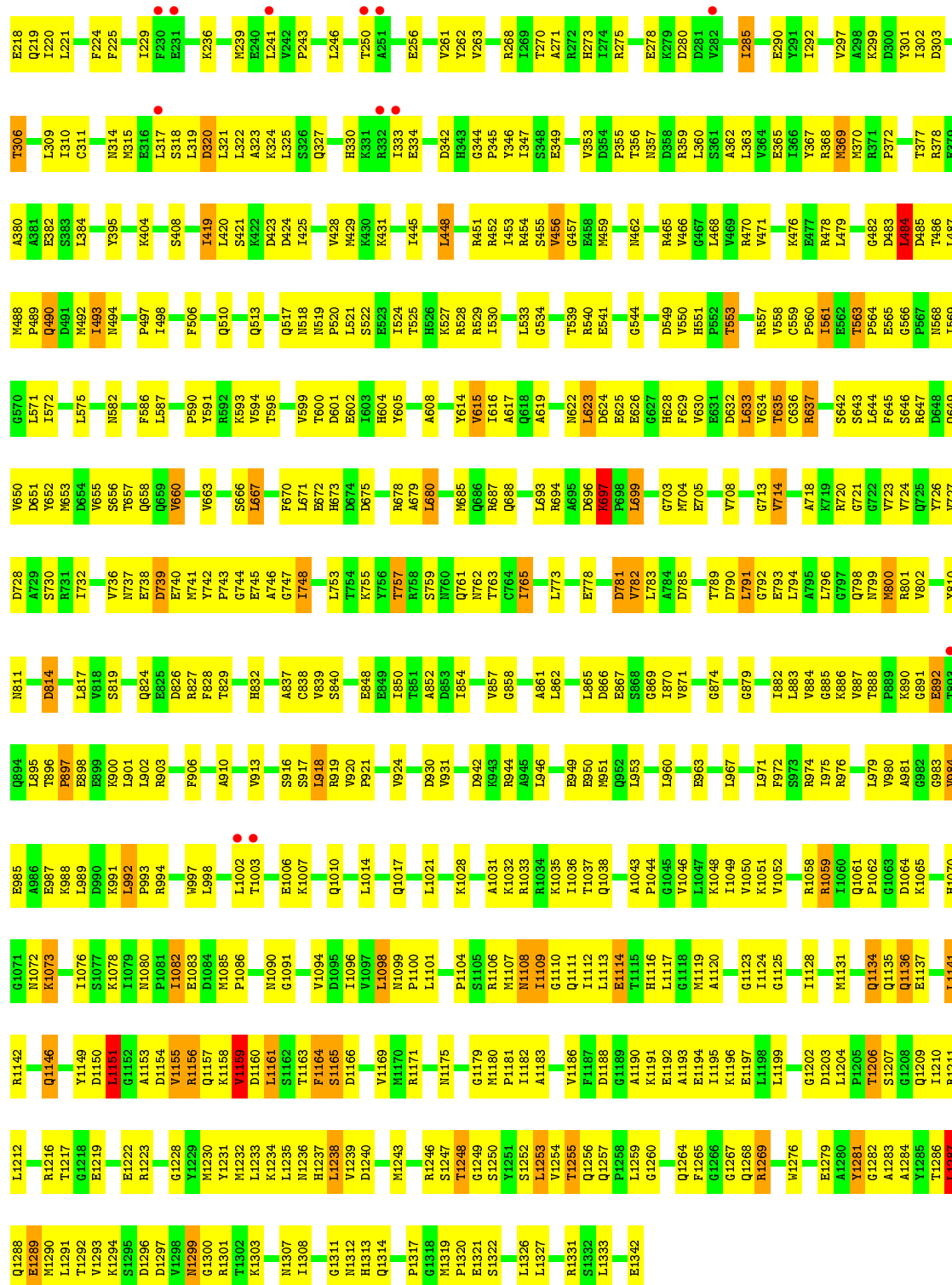


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			31	22	3	5	1		
8	J	1	Total	C	N	O	S	0	0
			31	22	3	5	1		

[illegible][illegible]

Chain C:

Item	Category	Percentage		
F136	Green	48%		
V137	Green			
I138	Green			
M139	Green			
G140	Green			
R143	Green			
V146	Green		46%	
S147	Green			
Q148	Green			
L149	Green			
H150	Green			
R151	Green			
F157	Green			
D158	Green			
S159	Green			
D160	Green			
K161	Green			
H165	Orange			6%
G168	Orange			
K169	Orange			
V170	Orange			
L171	Orange			
R175	Orange			
L176	Orange			
I177	Orange			
P178	Orange			
S182	Orange			
D185	Orange			
F188	Orange			
D189	Orange			
P190	Orange			
M193	Orange			
L194	Orange			
F195	Orange			
V196	Orange			
R197	Orange			
L198	Orange			
R201	Orange			
R202	Orange			
A206	Orange			
I208	Orange			
L209	Orange			
L210	Orange			
R211	Orange			
Y215	Orange			



● Molecule 2: DNA-directed RNA polymerase subunit beta



G1282	T1206	E1143	K1078	W997	R919	F828	Y742	A665	T589	L511	W429	D354	L241	K181	E84
A1283	I1210	Q1146	I1079	L998	V920	T829	P743	S666	P590	S512	K430	P355	V242	G168	C85
Y1285	R1211	Q1150	M1080	E999	P921	T830	G744	L667	K583	Q513	K431	T356	P243	T91	T91
L1287	L1212	Y1149	I1082	L1002	V924	H332	A746	F670	T595	D516	I435	R359	R245	Y92	Y92
Q1288	G1215	D1151	D1084	T1003	D830	L836	I748	B672	D596	N518	D443	L360	L246	L171	P95
L1289	R1216	G1152	M1085	T1004	V931	V839	Y751	H673	G597	N519	D444	S361	T250	W172	L96
M1290	G1217	A1153	P1086	E1005	Q932	V839	Y751	A676	T600	S522	I445	V364	R268	A174	R97
L1291	G1218	D1154	E1006	E1006	V933	L845	K755	R677	D601	S522	L448	V364	I269	R175	V98
L1292	E1219	V1155	Y1087	K1007	F934	L845	K755	R677	E602	S522	L448	V364	I269	I176	K99
K1293	Q1220	R1156	G1091	Q1008	R1156	L845	K755	R677	E602	S522	L448	V364	I269	I177	Y105
L1294	F1221	K1157	V1094	N1009	I341	E848	Y756	R678	T603	S523	R451	L366	R272	P178	Y105
S1295	E1222	K1158	D1095	Q1010	D942	E849	Y756	R678	T603	S523	R451	L366	H273	E106	E106
D1296	R1223	V1159	L1011	R943	K943	T850	R757	L880	H604	T525	R452	T367	H273	R107	R107
L1297	P1224	I1096	E1012	R944	R944	T851	S759	G682	H605	H526	V456	M369	L277	E108	E108
V1298	L1125	L1161	V1097	A945	A945	A852	I765	G682	S607	R528	Q457	N370	L277	A109	A109
L1299	T1226	S1162	L1098	L946	L946	D853	I765	M685	A608	R529	W462	P375	V282	D185	P110
G1300	V1227	T1163	M1099	E947	E947	I854	P769	Q686	A609	I530	R465	P376	K283	F186	E111
R1301	G1228	F1164	P1100	L945	L945	P855	C770	R687	E610	I530	R466	P376	L284	E187	E111
T1302	Y1229	S1165	L1101	Q1017	E949	N856	C770	Q688	E611	I530	R466	P376	L284	E187	E111
K1303	M1230	D1166	G1102	Y1018	V857	V857	S772	Q688	E611	I530	R466	P376	L284	E187	E111
M1304	Y1231	V1103	V1103	Q952	Q952	L862	G774	T692	V614	L538	R465	P376	L284	E187	E111
Y1305	K1234	V1169	R1106	K1022	D959	L862	G774	T692	V614	L538	R465	P376	L284	E187	E111
K1306	L1235	R1171	M1107	H1023	D959	E867	E775	D636	V615	T539	R465	P376	L284	E187	E111
N1307	L1235	R1171	M1107	H1023	D959	E867	E775	D636	V615	T539	R465	P376	L284	E187	E111
I1308	L1235	R1171	M1107	H1023	D959	E867	E775	D636	V615	T539	R465	P376	L284	E187	E111
V1309	L1235	R1171	M1107	H1023	D959	E867	E775	D636	V615	T539	R465	P376	L284	E187	E111
N1312	L1235	R1171	M1107	H1023	D959	E867	E775	D636	V615	T539	R465	P376	L284	E187	E111
H1313	L1235	R1171	M1107	H1023	D959	E867	E775	D636	V615	T539	R465	P376	L284	E187	E111
Q1314	L1235	R1171	M1107	H1023	D959	E867	E775	D636	V615	T539	R465	P376	L284	E187	E111
E1321	R1246	G1179	R1033	G970	E969	L833	E793	E705	D632	R557	R478	F390	L319	A206	P128
S1322	S1247	M1180	R1034	L971	L971	G885	A795	E705	D632	R557	R478	F390	L319	A206	P128
F1323	T1248	P1181	K1035	F972	F972	K886	L796	T715	L633	R558	R478	F390	L319	A206	P128
L1326	L1254	I1182	G1118	S973	S973	V887	G797	A716	T635	P560	G432	D395	L321	I208	M130
L1327	V1254	A1183	M1119	R974	R974	T888	Q793	V717	C636	I561	D433	L397	L322	I209	T131
R1331	Q1257	F1187	K1123	Q1037	Q1037	P899	W799	A718	R637	E562	D484	S398	K324	L210	D132
L1333	P1258	D1188	I1124	Q1038	Q1038	R890	R800	K719	F645	T563	D485	G401	L325	A212	T135
E1340	G1260	A1190	G1125	V1046	V1046	E891	R801	R720	S646	P564	T486	R402	Q327	L213	F136
D1341	G1261	K1191	I1128	I1049	I1049	P897	Y726	Q725	Q649	G570	P489	F405	H330	Q219	I138
E1342	K1262	E1192	M1129	G983	G983	E988	F812	Y727	D651	I572	D491	L409	K331	L220	N139
Q1264	A1263	E1194	M1131	L1054	L1054	R903	E813	D728	V652	M653	T493	I414	T335	K227	S147
F1265	F1265	I1195	L1132	R1059	R1059	R903	E813	A729	D654	S576	D495	G416	F337	F230	Q148
R1269	R1269	K1196	K1133	E987	E987	E908	S815	I732	V655	A579	K496	I419	T338	E231	L149
E1274	E1274	L1198	Q1134	R988	R988	R909	S815	V733	S656	A579	P497	T419	T338	E231	H150
V1275	V1275	L1199	Q1135	A910	A910	A910	S815	V733	S656	A579	P497	T419	T338	E231	R151
W1276	W1276	K1200	Q1136	D990	D990	W913	V818	K735	Q658	Q580	S499	L420	D342	R233	S152
G1202	G1202	L1201	V1138	L992	L992	K914	S819	V736	Q659	N582	S499	L420	D342	R233	P153
D1203	D1203	A1139	L1140	P993	P993	D915	E820	W737	V660	G585	V502	K422	G344	N235	F156
L1204	L1204	K1140	R1141	R994	R994	S916	Q824	E738	V661	F586	K503	D423	P345	L237	F157
P1205	P1205	R1142	L1142	S1077	S1077	S917	E740	D739	V663	F587	F506	I425	Y346	Q238	D158
						L918	R827	M741	G664	E588		V428	L351	E240	D160

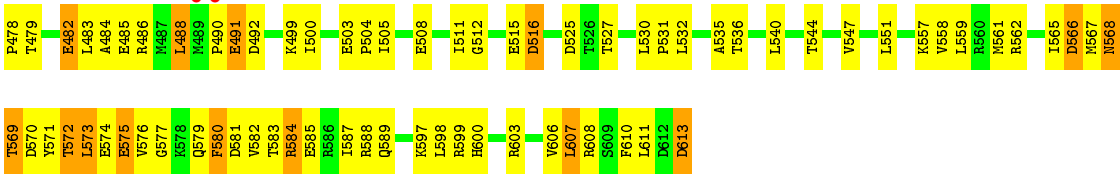
● Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 

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







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.10Å 206.44Å 307.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.57 31.02 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.96-3.57) 92.3 (31.02-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.217 , 0.252 0.264 , 0.279	Depositor DCC
R_{free} test set	2000 reflections (1.56%)	DCC
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 133164 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55782	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4C6, ZN, 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	0.80	0/2524	0.91	2/3421 (0.1%)
1	B	0.86	3/1697 (0.2%)	0.97	4/2300 (0.2%)
1	G	0.80	0/1777	0.92	1/2408 (0.0%)
1	H	0.83	1/1681 (0.1%)	0.94	1/2278 (0.0%)
2	C	0.84	1/10739 (0.0%)	0.89	9/14489 (0.1%)
2	I	0.79	2/10735 (0.0%)	0.87	10/14484 (0.1%)
3	D	0.90	6/9188 (0.1%)	0.95	18/12404 (0.1%)
3	J	0.78	2/9128 (0.0%)	0.89	10/12322 (0.1%)
4	E	0.73	0/693	0.75	0/935
4	K	1.03	0/629	0.89	0/847
5	F	0.83	1/3864 (0.0%)	0.87	3/5194 (0.1%)
5	L	0.83	1/3872 (0.0%)	0.83	2/5205 (0.0%)
All	All	0.83	17/56527 (0.0%)	0.90	60/76287 (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
2	C	0	3
2	I	0	4
3	D	0	2
3	J	0	1
5	F	0	1
All	All	0	11

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	799	ARG	CB-CG	-10.16	1.25	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	339	ARG	CZ-NH2	8.46	1.44	1.33
3	D	799	ARG	CG-CD	8.42	1.73	1.51
2	I	1296	ASP	CG-OD2	8.26	1.44	1.25
3	D	339	ARG	CB-CG	-8.08	1.30	1.52

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1269	ARG	NE-CZ-NH1	15.48	128.04	120.30
2	I	1269	ARG	NE-CZ-NH2	-11.03	114.79	120.30
2	I	484	LEU	CA-CB-CG	9.30	136.69	115.30
2	I	1269	ARG	CD-NE-CZ	9.27	136.57	123.60
2	C	1161	LEU	CA-CB-CG	-9.26	94.01	115.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	1264	GLN	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide

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	2490	0	2542	204	0
1	B	1677	0	1703	105	0
1	G	1755	0	1773	122	0
1	H	1662	0	1687	131	0
2	C	10570	0	10582	606	0
2	I	10566	0	10576	626	0
3	D	9050	0	9218	641	0
3	J	8990	0	9173	595	0
4	E	691	0	695	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	47	0
5	F	3813	0	3880	203	0
5	L	3821	0	3884	244	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	31	0	25	1	0
8	J	31	0	25	2	0
All	All	55782	0	56397	3255	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 29.

The worst 5 of 3255 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:G:190:ALA:HB2	1:G:200:LYS:HB2	1.29	1.14
1:A:45:ARG:HG2	1:B:38:THR:HB	1.31	1.12
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.30	1.08
2:I:1269:ARG:HD3	3:J:343:LEU:HD21	1.35	1.08
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.17	1.07

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	317/329 (96%)	243 (77%)	48 (15%)	26 (8%)	1 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/329 (65%)	193 (91%)	15 (7%)	5 (2%)	8	50
1	G	225/329 (68%)	195 (87%)	21 (9%)	9 (4%)	4	35
1	H	212/329 (64%)	193 (91%)	15 (7%)	4 (2%)	10	53
2	C	1338/1342 (100%)	1210 (90%)	111 (8%)	17 (1%)	15	61
2	I	1338/1342 (100%)	1207 (90%)	112 (8%)	19 (1%)	14	59
3	D	1157/1407 (82%)	1031 (89%)	101 (9%)	25 (2%)	8	51
3	J	1146/1407 (81%)	1032 (90%)	92 (8%)	22 (2%)	10	53
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	8	50
4	K	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	15	61
5	F	462/613 (75%)	424 (92%)	30 (6%)	8 (2%)	11	55
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	11	55
All	All	7035/8222 (86%)	6307 (90%)	582 (8%)	146 (2%)	9	52

5 of 146 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	107	ILE
1	A	114	ASP
1	A	136	GLU
1	A	195	ARG

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	278/286 (97%)	231 (83%)	47 (17%)	2	18
1	B	186/286 (65%)	172 (92%)	14 (8%)	17	57
1	G	193/286 (68%)	170 (88%)	23 (12%)	6	34
1	H	183/286 (64%)	170 (93%)	13 (7%)	18	59
2	C	1155/1157 (100%)	1048 (91%)	107 (9%)	11	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1154/1157 (100%)	1055 (91%)	99 (9%)	13	51
3	D	964/1168 (82%)	867 (90%)	97 (10%)	9	43
3	J	962/1168 (82%)	869 (90%)	93 (10%)	10	45
4	E	72/75 (96%)	67 (93%)	5 (7%)	19	60
4	K	67/75 (89%)	63 (94%)	4 (6%)	24	65
5	F	417/540 (77%)	376 (90%)	41 (10%)	10	44
5	L	418/540 (77%)	378 (90%)	40 (10%)	10	46
All	All	6049/7024 (86%)	5466 (90%)	583 (10%)	10	46

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1361	THR
1	G	168	ILE
3	J	1366	HIS
5	F	98	VAL
5	F	529	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	132	HIS
2	I	1038	GLN
4	K	7	GLN
2	I	139	ASN
2	I	658	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 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	$\# Z > 2$
8	4C6	D	2004	-	31,34,34	1.12	3 (9%)	39,51,51	0.80	1 (2%)
8	4C6	J	2004	-	31,34,34	0.72	0	39,51,51	1.22	4 (10%)

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
8	4C6	D	2004	-	-	0/7/45/45	0/3/4/4
8	4C6	J	2004	-	-	0/7/45/45	0/3/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C6	C2-S	-4.32	1.71	1.79
8	D	2004	4C6	S-N	-2.11	1.60	1.64
8	D	2004	4C6	C4-C3	-2.07	1.46	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	2004	4C6	C3-C2-C5	-3.93	104.58	107.52
8	D	2004	4C6	C3-C2-C5	-2.99	105.28	107.52
8	J	2004	4C6	C7-C21-C	-2.69	85.26	88.13
8	J	2004	4C6	C7-C1-N	2.55	135.43	130.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	2004	4C6	O3-S-C2	2.69	112.70	108.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C6	1	0
8	J	2004	4C6	2	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 ⓘ

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	319/329 (96%)	-0.30	5 (1%) 74 65	105, 138, 176, 185	0
1	B	217/329 (65%)	-0.13	4 (1%) 71 62	114, 172, 192, 198	0
1	G	227/329 (68%)	-0.35	1 (0%) 93 90	138, 159, 175, 192	0
1	H	216/329 (65%)	-0.04	6 (2%) 56 46	130, 174, 192, 201	0
2	C	1340/1342 (99%)	-0.34	13 (0%) 84 77	88, 126, 202, 228	0
2	I	1340/1342 (99%)	-0.16	35 (2%) 59 49	108, 154, 212, 314	0
3	D	1163/1407 (82%)	-0.33	3 (0%) 94 92	90, 119, 164, 197	0
3	J	1152/1407 (81%)	-0.23	10 (0%) 85 79	103, 137, 181, 211	0
4	E	89/91 (97%)	-0.20	0 100 100	129, 159, 178, 184	0
4	K	79/91 (86%)	0.66	8 (10%) 9 8	186, 221, 249, 254	0
5	F	468/613 (76%)	-0.21	15 (3%) 51 41	113, 159, 233, 249	0
5	L	469/613 (76%)	-0.18	12 (2%) 59 49	127, 168, 244, 260	0
All	All	7079/8222 (86%)	-0.24	112 (1%) 74 65	88, 143, 205, 314	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.1
2	I	1003	THR	7.1
5	F	167	ASP	5.6
2	I	1002	LEU	5.1
2	I	1004	ASP	5.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
8	4C6	D	2004	31/31	0.97	0.34	2.36	127,127,127,127	0
8	4C6	J	2004	31/31	0.95	0.32	1.45	127,127,128,141	0
7	ZN	D	2003	1/1	0.99	0.22	0.54	127,127,127,127	0
7	ZN	J	2003	1/1	0.96	0.20	-0.02	127,127,127,127	0
7	ZN	D	2002	1/1	0.98	0.18	-0.34	164,164,164,164	0
7	ZN	J	2002	1/1	0.97	0.12	-1.08	190,190,190,190	0
6	MG	D	2001	1/1	0.93	0.27	-	127,127,127,127	0
6	MG	C	1401	1/1	0.86	0.35	-	127,127,127,127	0
6	MG	J	2001	1/1	0.95	0.23	-	127,127,127,127	0
6	MG	I	1401	1/1	0.85	0.37	-	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.