



Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 12:17 AM EST

PDB ID : 6DQS
EMDB ID : EMD-7983
Title : Class 3 IP3-bound human type 3 1,4,5-inositol trisphosphate receptor
Authors : Hite, R.K.; Paknejad, N.
Deposited on : 2018-06-11
Resolution : 4.12 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

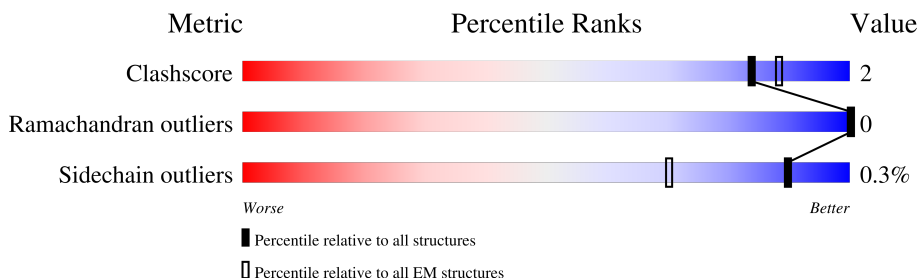
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.12 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2671	<div> <div>43%</div> <div>76%6%18%</div> </div>
1	B	2671	<div> <div>29%</div> <div>77%5%18%</div> </div>
1	C	2671	<div> <div>37%</div> <div>76%6%18%</div> </div>
1	D	2671	<div> <div>52%</div> <div>76%6%18%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 139350 atoms, of which 69675 are hydrogens and 0 are deuteriums.

In the tables below, 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.

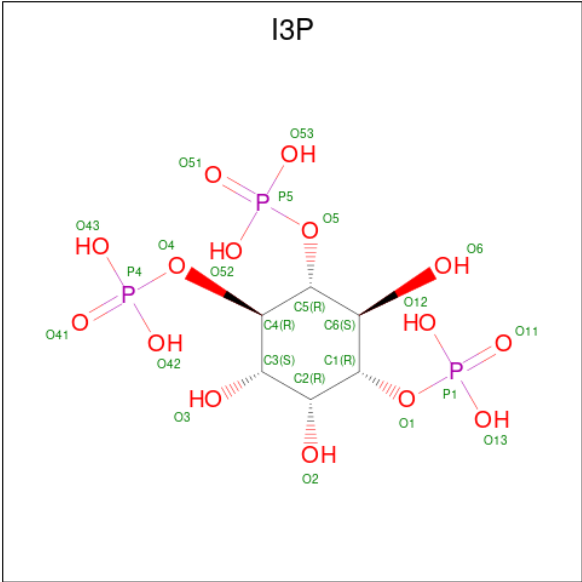
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2186	Total	C	H	N	O	S	0	0
			34696	11058	17351	2985	3199	103		
1	B	2186	Total	C	H	N	O	S	0	0
			34697	11058	17352	2985	3199	103		
1	C	2186	Total	C	H	N	O	S	0	0
			34694	11058	17349	2985	3199	103		
1	D	2192	Total	C	H	N	O	S	0	0
			35127	11194	17587	3005	3235	106		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).

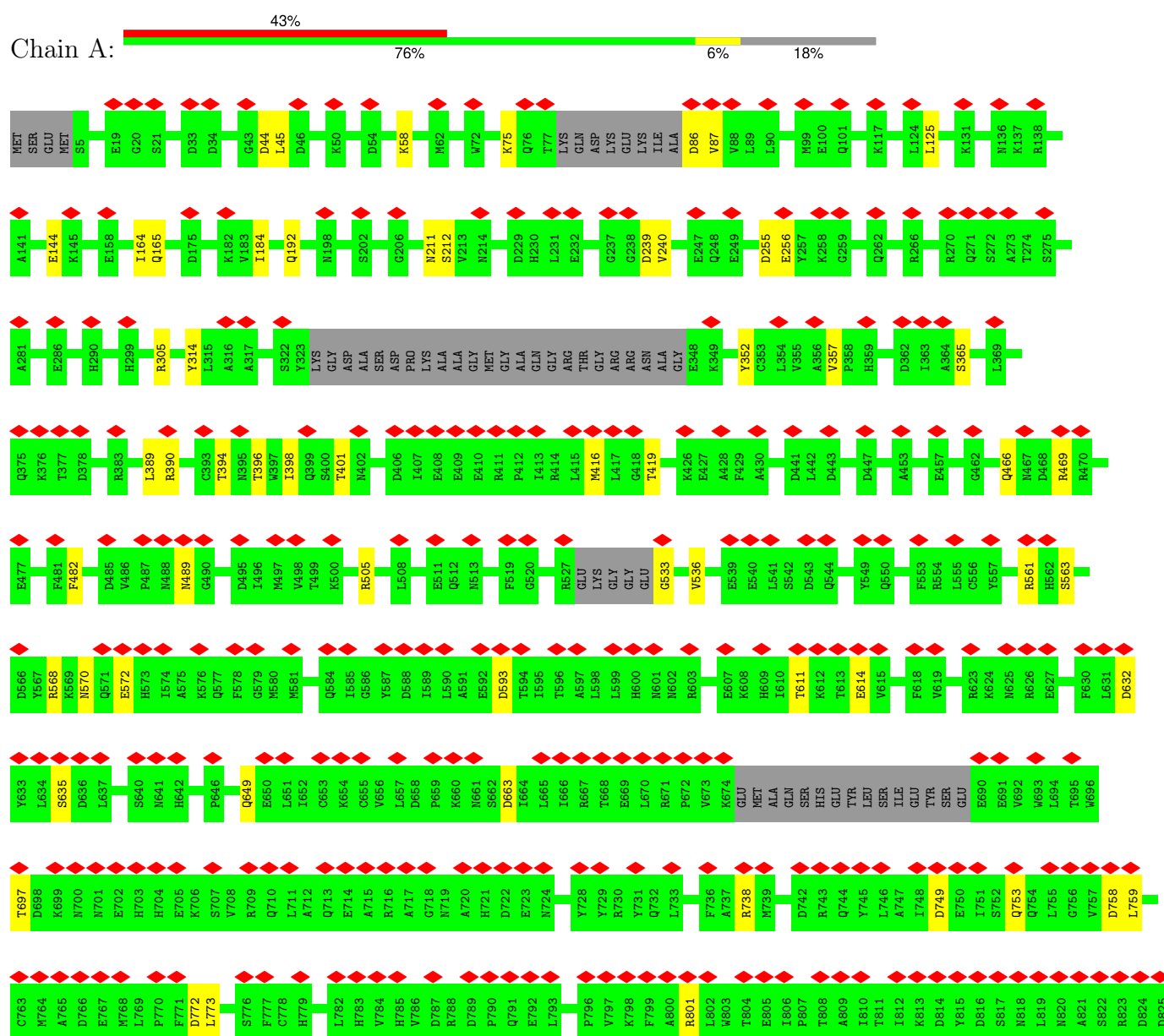


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

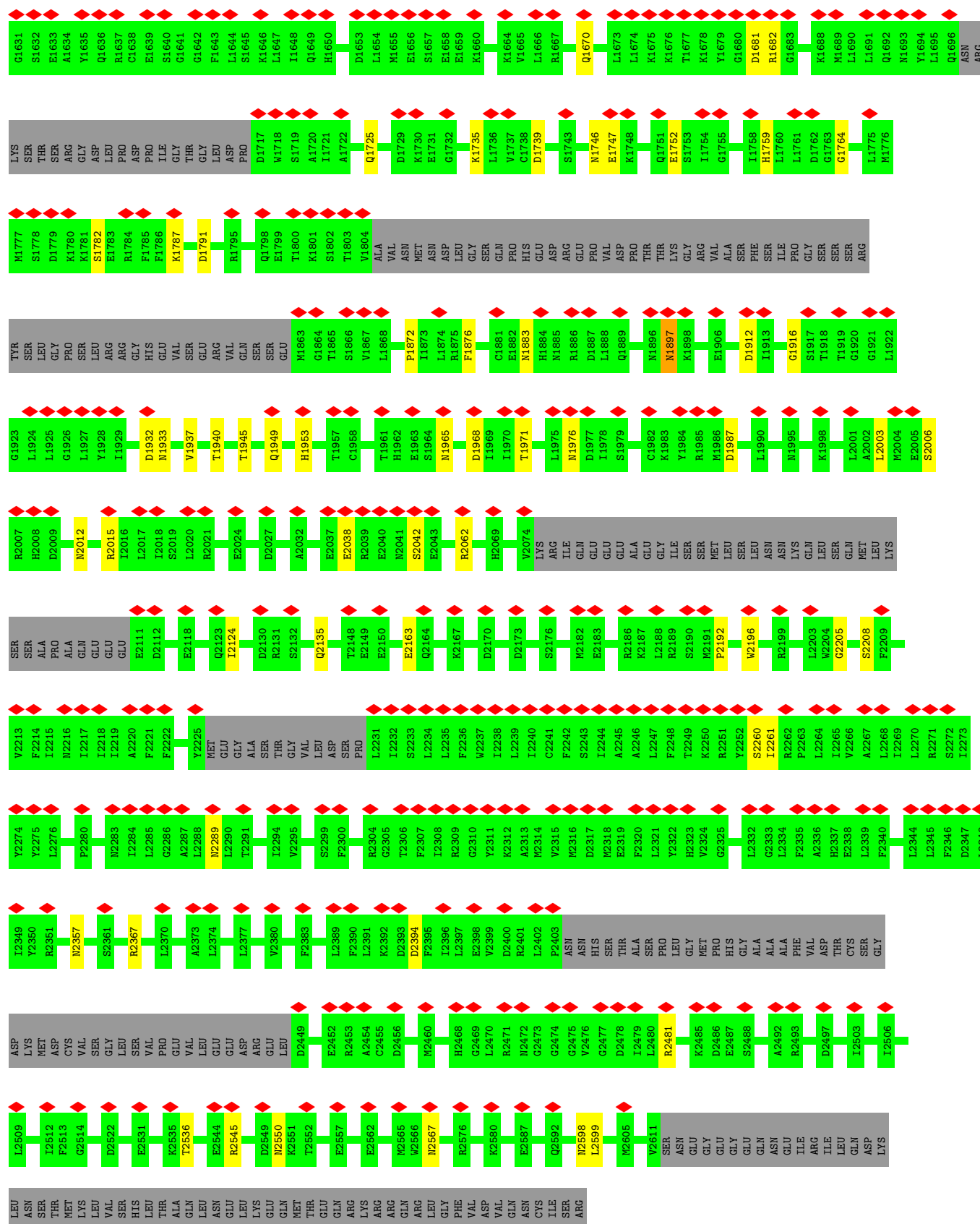
3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

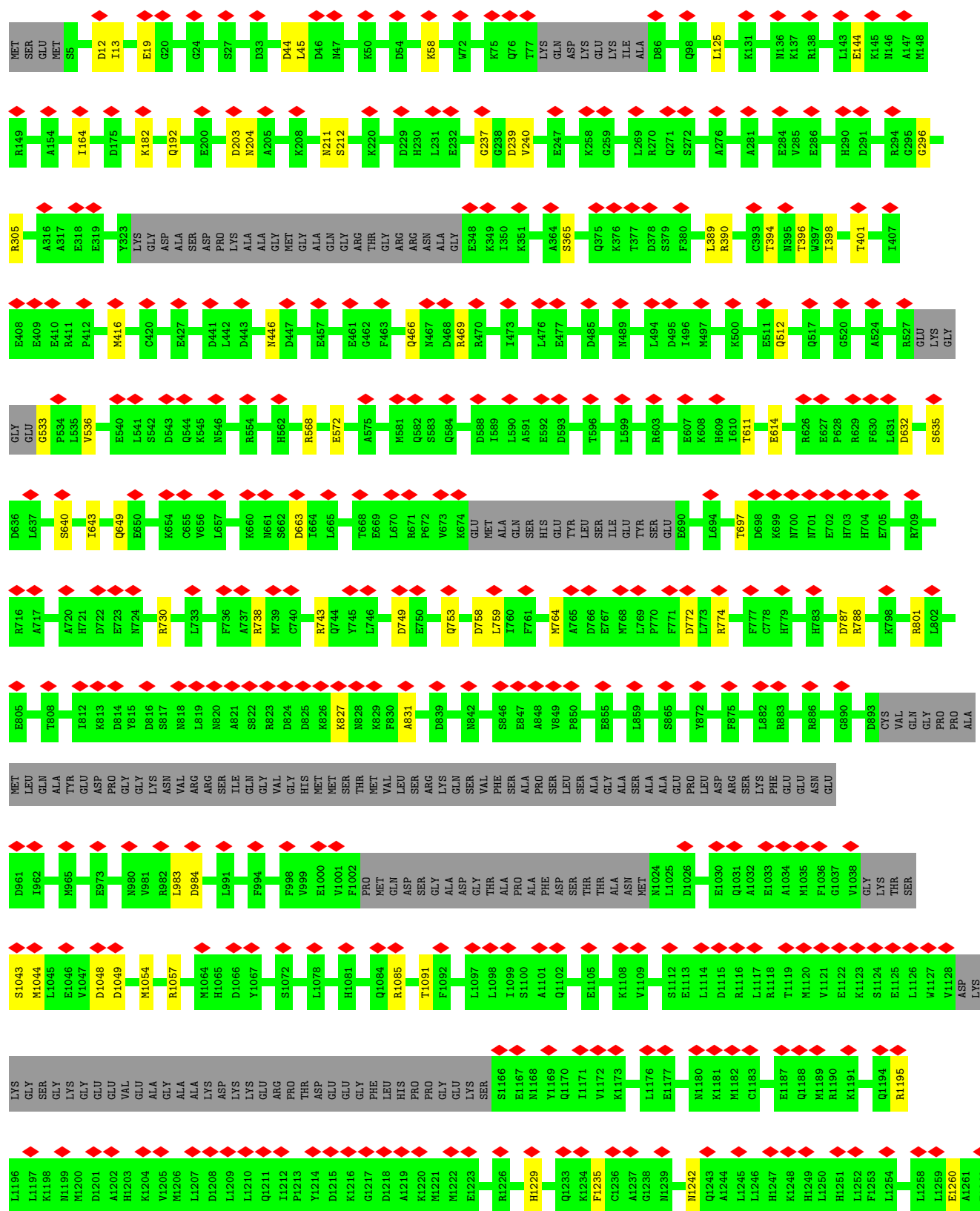
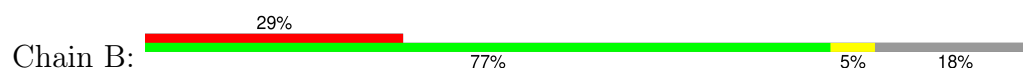
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

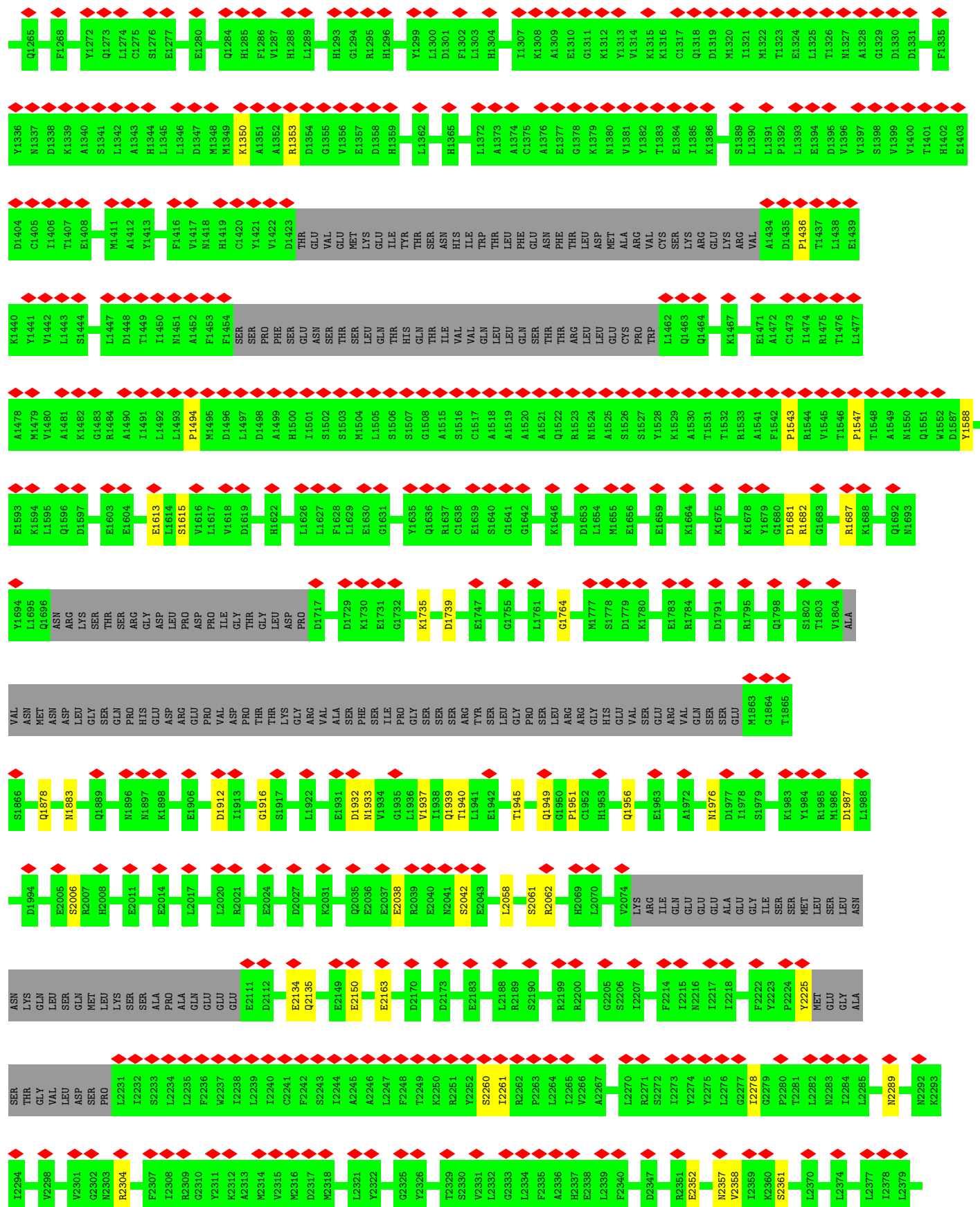


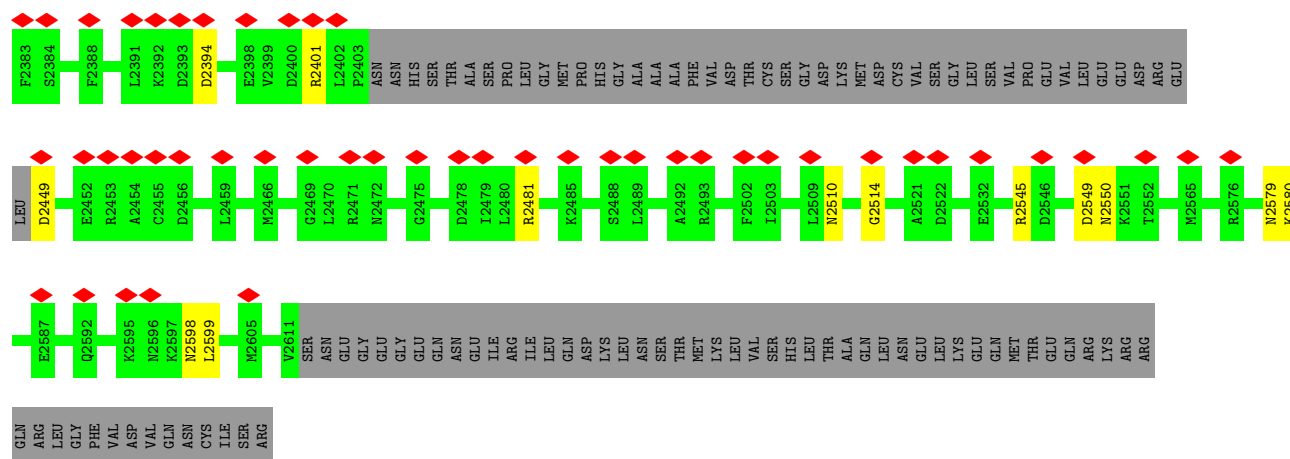
A1525	S1526	S1527	Y1528	K1529	A1530	T1531	T1532	Q1463	Q1464	Q1465	F1542	P1543	R1544	V1545	T1546	P1547	T1548	A1549	M1550	Q1551	W1552	D1587	Y1588	K1589	M1590	I1591	I1592	E1593	K1594	L1595	Q1596	I1491	D1597	I1598	I1599	T1600	A1601	L1602	E1603	E1604	R1605	L1606	V1610	Q1611	A1612	E1613	S1615	D1619	V1620	L1621	H1622	W1623	L1626	L1627	F1628	L1629	E1630																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
THR	ARG	LEU	LEU	GLU	CYS	PRO	TRP	L1462	Q1463	Q1464	Q1465	H1466	K1467	G1468	S1469	V1470	E1471	A1472	C1473	R1474	T1475	R1476	L1477	A1478	M1479	V1480	A1481	K1482	G1483	R1484	A1490	I1491	L1492	L1493	P1494	M1495	D1496	L1497	D1498	A1499	H1500	I1501	S1502	S1503	M1504	L1505	S1506	S1507	G1508	A1515	S1516	C1517	A1518	A1519	A1520	Q1522	R1523	N1524																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
LEU	ASP	MET	ARG	ALA	VAL	CYS	SER	LYS	GLY	ARG	VAL	A1434	D1435	P1436	T1437	L1438	E1439	K1440	Y1441	V1442	L1443	S1444	V1445	V1446	L1447	D1448	T1449	I1450	N1451	A1452	F1453	F1454	SER	SER	PRO	PHE	SER	GLU	ASN	SER	THR	SER	LEU	GLN	THR	HIS	GLN	THR	ILE	THR	VAL	VAL	GLN	LEU	GLN	SER	THR	D1619	V1620	L1621	H1622	W1623	L1626	L1627	F1628	L1629	E1630																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
K1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	L1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	L1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1



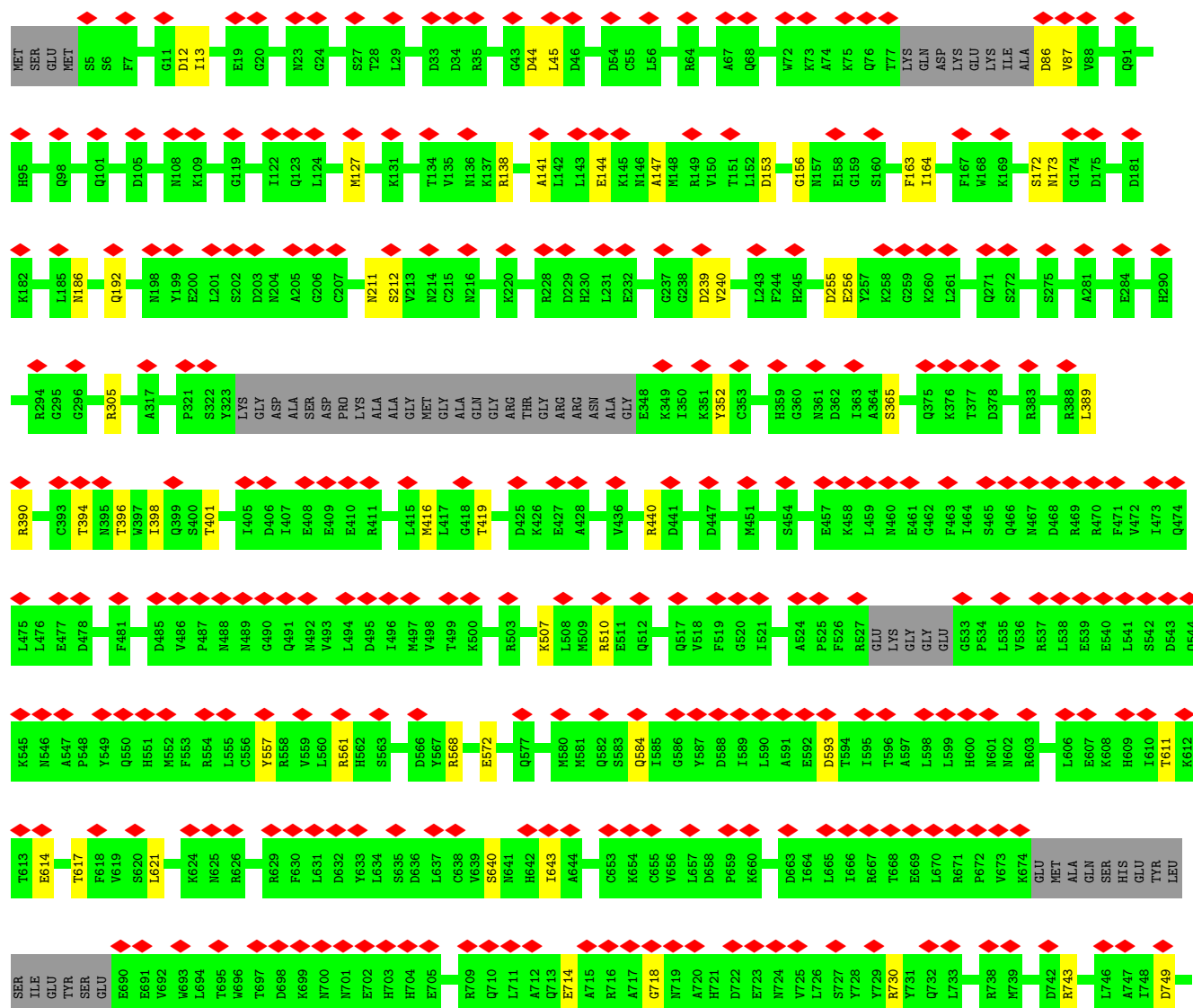
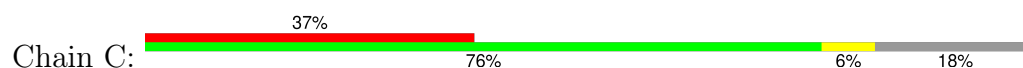
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







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SER	ARG	LYS	GLN	SER	VAL	PHE	SER	ALA	ALA	PRO	SER	LEU	SER	ALA	GLY	ALA	SER	ALA	ALA	GLU	PRO	ASP	ARG	SER	LYS	PHE	GLU	GLU	ASN	GLU	D961	I962	V963	V964	N965	E966	T967	K968	L969	K970	I971	L972	E973	I974	L975	Q976	F977	I978	L979	N980	V981	R982	D984	Y985	R986	I987	S988	Y989			
H868	N869	L870	I871	Y872	F873	G874	F875	Y876	S877	E880	L881	L882	R883	L884	T885	R886	L887	L888	I889	L892	D893	CYS	VAL	GLN	GLY	PRO	PRO	ALA	MET	LEU	GLN	ALA	TYR	GLU	ASP	PRO	GLY	LYS	ASN	VAL	ARG	ARG	SER	ILE	GLN	GLY	VAL	HIS	MET	MET	SER	THR	MET	VAL	LEU	S988	Y989				
T808	A809	I810	T811	L812	F813	D814	Y815	D816	S817	N818	L819	N820	A821	S822	R823	D824	D825	K826	K827	N828	K829	F830	A831	N832	T833	M834	E835	F836	V837	E838	D839	Y840	L841	N842	N843	V844	V845	S846	E847	A848	V849	F850	F851	A852	N853	E854	E855	K856	N857	K858	L859	T860	F861	E862	V863	V864	S865	L866	A867		
L746	A747	I748	D749	E750	L751	S752	Q753	Q754	L755	G756	T757	D758	L759	I760	F761	L762	C763	M764	A765	D766	E767	M768	L769	P770	F771	D772	A775	S776	F777	C778	H779	L780	H783	W784	H785	V786	D787	R788	D789	F790	Q791	E792	L793	A852	N853	T854	F796	K855	K856	N857	K858	L859	F861	E862	W803	T804	E805	I806	S865	L866	A867
R626	E627	F628	R629	F630	L631	D632	F633	L634	S635	D636	L637	C638	Y639	S640	R641	L642	I643	A644	L645	P646	T648	Q649	E650	L651	L652	C653	K654	C655	V656	L657	D658	P659	K660	N661	S662	D663	L664	L665	L666	R667	T668	E669	L670	R671	F672	VAL	LYS	GLU	MET	ALA	GLN	SER	HIS	TYR	LEU	SER	ILE				
D566	Y567	R568	K569	M570	Q571	E572	H573	L574	A575	K576	Q577	F578	G579	M580	Q582	S583	Q584	L585	G586	Y587	D588	L589	L590	A591	E592	D593	T594	L595	T596	A597	L598	L599	H600	N601	N602	R603	K604	L605	L606	E607	K608	H609	L610	T611	K612	E613	E614	V615	E616	T617	F618	V619	S620	L621	V622	R623	K624	H625			
E504	R505	D506	K507	L508	M509	Q512	N513	I514	L515	K516	Q517	V518	F519	G520	I521	L522	K523	A524	P525	F526	R527	GLU	LYS	GLY	GLY	G533	P534	D535	T536	L537	E538	E539	E540	L541	S542	D543	Q544	K545	N546	A547	P548	Y549	Q550	H551	M552	F553	R554	L555	C556	Y557	R558	R561	H562	S563	Q564	E565					
D443	F444	A445	N446	D447	A448	S449	L452	A453	S454	A455	V456	K458	L459	N460	E461	G462	F463	I464	S465	Q466	N467	D468	R469	R470	F471	V472	L473	Q474	L475	L476	E477	D478	L479	V480	F481	F482	V483	S484	D485	V486	F487	N488	M489	G490	Q491	N492	V493	L494	D495	I496	M497	V498	T499	K500	P501	N502	R503				
N361	D362	I363	A364	S365	L366	F367	D370	L374	Q375	K376	D377	S378	S379	F380	L389	R390	C393	T394	N395	I398	Q399	S400	T401	N402	V403	D406	I407	E408	E410	R411	M416	L417	G418	T419	C420	E424	D425	K426	E427	A428	F429	A430	S433	V436	R440	D441	L442														
H290	D291	R294	G295	G296	A297	R305	L309	G312	N313	Y314	V315	N316	A317	E318	E319	N320	P321	S322	L323	LYS	GLY	ASP	ALA	SER	ASP	PRO	LYS	ALA	ALA	GLY	THR	GLY	ARG	GLY	ARG	ASN	ALA	GLY	E348	K349	I350	K351	L354	V355	A356	V357	P358	H359	G360												
Y199	E200	L201	D203	N204	A205	G206	K208	E209	N211	S212	V213	N214	K220	F224	M225	H230	K236	G237	G238	D239	V240	V241	R242	H245	A246	E247	Q248	L252	D255	K258	G259	K260	L261	R266	L269	R270	Q271	S272	A273	T274	S275	A281	E284																		
Q101	K102	D105	N108	I122	Q123	L124	L125	H126	M127	K128	V123	S129	N130	K131	N136	K137	R138	L139	P140	A141	L142	E144	K145	N146	A147	D153	A154	T155	G156	N157	E158	L162	F163	I164	Q165	K169	V177	G180	D181	K182	V183	I184	L185	N189	Q192	N198															
MET	SER	GLU	MET	S5	G11	D12	L16	Y17	E19	G20	S21	V22	W23	S27	L31	V32	D33	D34	E39	G43	D44	L45	D46	K50	D54	K58	W72	K73	A74	K75	Q76	T77	LYS	GLN	ASP	LYS	GLU	ILE	ALA	D86	V87	V88	L89	L90	Q91	Q98															

L990	L991	G1051	G1052	G1053	M1054	F1055	L1056	R1057	V1058	L1059	I1060	H1061	L1062	T1063	M1064	H1065	D1066	Y1067	A1068											V1071	S1072	G1073	A1074	L1075	Q1076	L1077	L1078	F1079	K1080	H1081	M1082	L1083	D1084	R1085	Q1086	I1087	A1088	M1089	H1090	T1091	F1092	K1093	Q1094	Q1095	Q1096	L1097	L1098	I1099	S1100	A1101	Q1102	D1103	V1104	E1105	N1106	Y1107	K1108	V1109	I1110	
E1050	G1051	G1052	R1053	M1054	F1055	L1056	R1057	V1058	L1059	I1060	H1061	L1062	T1063	M1064	H1065	D1066	Y1067	A1068											V1071	S1072	G1073	A1074	L1075	Q1076	L1077	L1078	F1079	K1080	H1081	M1082	L1083	D1084	R1085	Q1086	I1087	A1088	M1089	H1090	T1091	F1092	K1093	Q1094	Q1095	Q1096	L1097	L1098	I1099	S1100	A1101	Q1102	D1103	V1104	E1105	N1106	Y1107	K1108	V1109	I1110		
K1111	S1112	Q1113	L1114	D1115	R1116	L1117	R1118	T1119	M1120	V1121	E1122	K1123	S1124	E1125	L1126	W1127	V1128	D1129											L1129	L1130	G1131	L1132	F1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	Q1170
I1171	V1172	K1173	G1174	L1175	L1176	E1177	R1178	L1179	M1180	K1181	M1182	C1183	G1184	V1185	G1186	E1187	Q1188	M1189	R1190	K1191	L1192	Q1193	Q1194	R1195	L1196	L1197	L1198	M1199	M1200	D1201	A1202	H1203	K1204	V1205	M1206	L1207	D1208	L1209	L1210	Q1211	I1212	P1213	Y1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	I1224	L1225	R1226	Y1227	T1228	H1229	Q1230											
F1231	L1232	Q1233	K1234	F1235	C1236	A1237	G1238	N1239	P1240	G1241	N1242	Q1243	A1244	L1245	L1246	H1247	K1248	H1249	L1250	H1251	K1252	F1253	L1254	T1255	P1256	C1257	L1258	L1259	E1260	A1261	E1262	T1263	M1264	Q1265	H1266	L1267	F1268	L1269	N1270	M1271	Y1272	Q1273	L1274	C1275	D1276	E1277	I1278	S1279	E1280	P1281	V1282	L1283	Q1284	H1285	L1286	V1287	L1288	L1289	L1290											
A1291	T1292	H1293	G1294	L1295	H1296	V1297	Q1298	L1299	L1300	D1301	F1302	L1303	H1304	T1305	V1306	L1307	K1308	A1309	E1310	G1311	K1312	L1313	V1314	K1315	K1316	C1317	Q1318	D1319	M1320	I1321	M1322	T1323	E1324	L1325	T1326	M1327	A1328	G1329	D1330	D1331	V1332	L1333	V1334	F1335	Y1336	M1337	D1338	K1339	A1340	S1341	L1342	A1343	H1344	L1345	L1346	D1347	M1348	M1349	K1350											
A1351	A1352	R1353	D1354	G1355	V1356	E1357	D1358	H1359	S1360	P1361	L1362	M1363	Y1364	H1365	I1366	S1367	L1368	V1369	D1370	L1371	L1372	A1373	S1374	C1375	A1376	E1377	G1378	K1379	M1380	V1381	Y1382	L1383	E1384	I1385	K1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	D1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	T1406	I1407	E1408	V1409	K1410											
M1411	A1412	Y1413	V1414	M1415	F1416	V1417	N1418	H1419	C1420	Y1421	D1422	D1423	T1424	E1425	V1426	E1427	M1428	K1429	E1430	I1431	Y1432	T1433	S1434	M1435	H1436	I1437	V1438	L1439	T1440	F1441	A1442	M1443	F1444	T1445	L1446	D1447	M1448	A1449	R1450	V1451	C1452	S1453	K1454	L1455	GLU	LYS	ARG	VAL	ALA	ASP	PRO	T1463	L1464	E1465	K1466	Y1467	V1468	L1469	S1470											
V1471	V1472	L1473	D1474	T1475	I1476	N1477	A1478	F1479	F1480	S1481	S1482	P1483	PHE	SER	GLU	ASN	SER	SER	GLN	THR	HIS	GLN	THR	ILE	VAL	GLN	LEU	GLN	SER	THR	ARG	LEU	CYS	PRO	TRP	S1527	Y1528	K1529	A1530	H1531	T1532	R1533	A1541	F1542	P1543	R1544	V1545	T1546	P1547	A1490																				
M1491	V1492	A1493	K1494	G1495	R1496	A1497	I1498	L1499	L1500	P1501	M1502	D1503	L1504	D1505	A1506	H1507	I1508	SER	SER	MET	LEU	SER	GLY	A1515	S1516	C1517	A1518	A1519	A1520	A1521	Q1522	R1523	M1524	A1525	S1526	S1527	Y1528	K1529	A1530	H1531	T1532	R1533	A1541	F1542	P1543	R1544	V1545	T1546	P1547	A1490																				
I1591	I1592	E1593	K1594	L1595	Q1596	D1597	I1598	I1599	T1600	A1601	L1602	E1603	E1604	R1605	L1606	K1607	P1608	L1609	E1613	V1616	L1617	V1618	D1619	V1620	L1621	H1622	P1623	P1624	E1625	L1626	L1627	F1628	L1629	E1630	G1631	S1632	E1633	A1634	Y1635	Q1636	R1637	C1638	F1639	S1640	G1641	G1642	F1643	K1646	L1647	I1648	Q1649	H1650	T1651	K1652	D1653	L1654														
M1655	E1656	S1657	E1658	E1659	K1660	L1661	C1662	I1663	K1664	L1667	T1668	L1669	Q1670	Q1671	M1672	L1673	L1674	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	M1684	Q1685	K1688	M1689	L1690	L1691	Q1692	M1693	Y1694	L1695	Q1696	ASN	ARG	LYS	SER	THR	SER	ARG	GLY	ASP	LEU	PRO	ASP	PRO	ILE	GLY	THR	GLY	LEU	ASP	PRO	ASP														
W1718	S1719	A1720	A1723	C1726	R1727	L1728	D1729	K1730	E1731	G1732	A1733	T1734	K1735	C1738	D1739	T1742	S1743	T1744	K1745	M1746	E1747	I1754	G1755	I1758	L1761	D1762	G1763	G1764	E1767	I1768	K1770	S1771	F1772	H1773	M1774	L1775	M1776	M1777	S1778	D1779	K1780	K1781	S1782	E1783	R1784	F1785	F1786	K1787	D1791																					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	19.496	Depositor
Minimum map value	-12.071	Depositor
Average map value	-0.013	Depositor
Map value standard deviation	0.917	Depositor
Recommended contour level	3.93	Depositor
Map size (Å)	417.79202, 417.79202, 417.79202	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, I3P

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	0.25	0/17650	0.46	4/23851 (0.0%)
1	B	0.25	0/17650	0.46	4/23851 (0.0%)
1	C	0.25	0/17650	0.46	4/23851 (0.0%)
1	D	0.25	0/17856	0.46	3/24125 (0.0%)
All	All	0.25	0/70806	0.46	15/95678 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1547	PRO	N-CA-CB	5.73	110.18	103.30
1	D	1543	PRO	N-CA-CB	5.71	110.16	103.30
1	D	1547	PRO	N-CA-CB	5.71	110.16	103.30
1	B	1547	PRO	N-CA-CB	5.70	110.14	103.30
1	C	1547	PRO	N-CA-CB	5.69	110.12	103.30
1	A	1494	PRO	N-CA-CB	5.68	110.12	103.30
1	D	1501	PRO	N-CA-CB	5.67	110.11	103.30
1	A	1543	PRO	N-CA-CB	5.64	110.07	103.30
1	C	1494	PRO	N-CA-CB	5.64	110.07	103.30
1	C	1436	PRO	N-CA-CB	5.64	110.06	103.30
1	C	1543	PRO	N-CA-CB	5.58	110.00	103.30
1	B	1543	PRO	N-CA-CB	5.58	110.00	103.30
1	B	1436	PRO	N-CA-CB	5.51	109.92	103.30
1	B	1494	PRO	N-CA-CB	5.51	109.91	103.30
1	A	1436	PRO	N-CA-CB	5.39	109.76	103.30

There are no chirality outliers.

There are no planarity outliers.

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	17345	17351	17180	75	0
1	B	17345	17352	17181	69	0
1	C	17345	17349	17179	77	0
1	D	17540	17587	17485	92	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0
3	B	24	9	9	0	0
3	C	24	9	9	2	0
3	D	24	9	9	1	0
All	All	69675	69675	69061	305	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 2.

All (305) 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:A:801:ARG:NH2	1:A:984:ASP:OD1	2.19	0.76
1:B:144:GLU:OE2	1:B:211:ASN:ND2	2.21	0.74
1:A:2545:ARG:NH1	1:D:2163:GLU:O	2.20	0.74
1:C:510:ARG:NH2	3:C:3002:I3P:O52	2.21	0.73
1:B:749:ASP:O	1:B:753:GLN:NE2	2.22	0.73
1:D:144:GLU:OE2	1:D:211:ASN:ND2	2.21	0.73
1:A:1782:SER:OG	1:A:1897:ASN:OD1	2.05	0.73
1:C:144:GLU:OE2	1:C:211:ASN:ND2	2.22	0.73
1:B:192:GLN:O	1:B:212:SER:OG	2.07	0.73
1:C:2163:GLU:O	1:D:2545:ARG:NH1	2.22	0.72
1:A:144:GLU:OE2	1:A:211:ASN:ND2	2.22	0.72
1:A:192:GLN:O	1:A:212:SER:OG	2.08	0.71
1:A:1118:ARG:NH2	1:A:1200:MET:O	2.23	0.71
1:C:127:MET:O	1:C:440:ARG:NH2	2.23	0.71
1:A:749:ASP:O	1:A:753:GLN:NE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLN:O	1:C:212:SER:OG	2.09	0.70
1:A:568:ARG:NH2	1:A:572:GLU:OE2	2.25	0.70
1:B:2163:GLU:O	1:C:2545:ARG:NH1	2.24	0.70
1:A:649:GLN:NE2	1:A:738:ARG:O	2.25	0.70
1:A:2163:GLU:O	1:B:2545:ARG:NH1	2.25	0.70
1:C:2394:ASP:OD1	1:C:2481:ARG:NH2	2.25	0.69
1:A:401:THR:OG1	1:A:416:MET:O	2.10	0.69
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.26	0.69
1:C:568:ARG:NH2	1:C:572:GLU:OE2	2.24	0.69
1:C:2038:GLU:OE2	1:C:2042:SER:OG	2.09	0.69
1:D:1085:ARG:NH1	1:D:1613:GLU:OE2	2.25	0.69
1:B:2006:SER:OG	1:B:2134:GLU:OE1	2.06	0.69
1:D:192:GLN:O	1:D:212:SER:OG	2.09	0.69
1:A:1987:ASP:OD1	1:A:2042:SER:OG	2.07	0.69
1:C:1987:ASP:OD1	1:C:2042:SER:OG	2.07	0.69
1:C:749:ASP:O	1:C:753:GLN:NE2	2.26	0.69
1:D:533:GLY:N	1:D:536:VAL:O	2.26	0.69
1:B:1937:VAL:O	1:B:1940:THR:OG1	2.10	0.68
1:A:1735:LYS:NZ	1:A:1739:ASP:OD2	2.20	0.68
1:A:533:GLY:N	1:A:536:VAL:O	2.27	0.68
1:B:533:GLY:N	1:B:536:VAL:O	2.27	0.68
1:D:305:ARG:NH2	1:D:365:SER:O	2.25	0.68
1:B:1235:PHE:O	1:B:1242:ASN:ND2	2.26	0.68
1:C:827:LYS:O	1:C:831:ALA:N	2.27	0.68
1:A:1085:ARG:NH1	1:A:1613:GLU:OE2	2.26	0.67
1:B:446:ASN:ND2	1:B:512:GLN:OE1	2.27	0.67
1:B:611:THR:OG1	1:B:614:GLU:OE1	2.11	0.66
1:D:1956:GLN:NE2	1:D:2002:ALA:O	2.28	0.66
1:C:401:THR:OG1	1:C:416:MET:O	2.13	0.66
1:C:1968:ASP:O	1:C:1971:THR:OG1	2.13	0.66
1:D:572:GLU:O	1:D:576:LYS:NZ	2.28	0.66
1:D:1053:ARG:NH1	1:D:1694:TYR:O	2.29	0.66
1:C:1085:ARG:NH1	1:C:1613:GLU:OE2	2.29	0.66
1:C:2003:LEU:O	1:C:2012:ASN:ND2	2.30	0.65
1:C:561:ARG:NH1	1:C:593:ASP:O	2.30	0.65
1:C:2401:ARG:NE	1:C:2449:ASP:OD2	2.29	0.65
1:C:352:TYR:O	1:C:419:THR:OG1	2.13	0.64
1:D:305:ARG:NH2	1:D:365:SER:OG	2.30	0.64
1:B:389:LEU:HB2	1:B:398:ILE:HD12	1.80	0.63
1:A:2038:GLU:OE2	1:A:2042:SER:OG	2.15	0.63
1:A:838:GLU:O	1:A:842:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LEU:HB2	1:D:398:ILE:HD12	1.79	0.62
1:B:2401:ARG:NE	1:B:2449:ASP:OD2	2.32	0.62
1:D:1214:TYR:OH	1:D:1222:MET:SD	2.50	0.62
1:B:743:ARG:NH1	1:B:787:ASP:O	2.32	0.62
1:B:1987:ASP:OD1	1:B:2042:SER:OG	2.10	0.62
1:A:1725:GLN:NE2	1:A:1759:HIS:O	2.33	0.62
1:A:352:TYR:O	1:A:419:THR:OG1	2.13	0.62
1:B:401:THR:OG1	1:B:416:MET:O	2.18	0.61
1:B:568:ARG:NH2	1:B:572:GLU:OE2	2.33	0.61
1:C:1235:PHE:O	1:C:1242:ASN:ND2	2.33	0.61
1:B:1945:THR:O	1:B:1949:GLN:N	2.33	0.61
1:C:557:TYR:OH	1:C:584:GLN:OE1	2.17	0.61
1:C:2062:ARG:NH1	1:C:2135:GLN:OE1	2.34	0.60
1:A:1945:THR:O	1:A:1949:GLN:N	2.34	0.60
1:C:138:ARG:NH1	1:D:1425:GLU:O	2.34	0.60
1:C:389:LEU:HB2	1:C:398:ILE:HD12	1.84	0.60
1:C:1878:GLN:OE1	1:C:1939:GLN:NE2	2.35	0.59
1:C:1945:THR:O	1:C:1949:GLN:N	2.35	0.59
1:A:75:LYS:NZ	1:A:489:ASN:O	2.36	0.59
1:D:466:GLN:OE1	1:D:469:ARG:NH2	2.36	0.59
1:D:2394:ASP:OD1	1:D:2481:ARG:NH2	2.36	0.59
1:B:649:GLN:NE2	1:B:738:ARG:O	2.36	0.58
1:D:814:ASP:O	1:D:817:SER:OG	2.14	0.58
1:A:611:THR:OG1	1:A:614:GLU:OE1	2.11	0.58
1:B:632:ASP:O	1:B:635:SER:OG	2.16	0.58
1:B:2394:ASP:OD1	1:B:2481:ARG:NH2	2.37	0.58
1:B:1735:LYS:NZ	1:B:1739:ASP:OD2	2.32	0.58
1:D:153:ASP:OD2	1:D:156:GLY:N	2.36	0.58
1:B:1085:ARG:NH1	1:B:1613:GLU:OE2	2.37	0.58
1:C:1937:VAL:O	1:C:1940:THR:OG1	2.13	0.58
1:D:1391:LEU:O	1:D:1421:TYR:OH	2.21	0.58
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.37	0.57
1:B:2038:GLU:OE2	1:B:2042:SER:OG	2.21	0.57
1:A:1937:VAL:O	1:A:1940:THR:OG1	2.15	0.57
1:C:611:THR:OG1	1:C:614:GLU:OE1	2.14	0.56
1:D:1054:MET:SD	1:D:1057:ARG:NH2	2.78	0.56
1:D:1937:VAL:O	1:D:1940:THR:OG1	2.16	0.56
1:D:1890:ASN:OD1	1:D:1893:ARG:NH2	2.37	0.56
1:D:2125:GLU:OE1	1:D:2563:HIS:NE2	2.38	0.56
1:D:2369:ILE:HG23	1:D:2512:ILE:HG23	1.87	0.56
1:A:389:LEU:HB2	1:A:398:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1951:PRO:O	1:B:1956:GLN:NE2	2.38	0.56
1:C:1928:TYR:O	1:C:1933:ASN:ND2	2.39	0.56
1:A:1912:ASP:O	1:A:1916:GLY:N	2.38	0.56
1:A:561:ARG:NH1	1:A:593:ASP:O	2.39	0.56
1:C:806:ILE:O	1:C:995:LYS:NZ	2.25	0.56
1:C:1116:ARG:O	1:C:1119:THR:OG1	2.16	0.56
1:A:2205:GLY:O	1:A:2208:SER:OG	2.24	0.55
1:B:19:GLU:OE1	1:B:182:LYS:NZ	2.26	0.55
1:A:2003:LEU:O	1:A:2012:ASN:ND2	2.39	0.55
1:A:482:PHE:O	1:A:505:ARG:NH1	2.40	0.55
1:A:663:ASP:OD1	1:A:697:THR:OG1	2.22	0.55
1:A:2192:PRO:O	1:A:2196:TRP:N	2.40	0.55
1:D:2047:ARG:O	1:D:2051:HIS:ND1	2.40	0.54
1:B:2062:ARG:NH1	1:B:2135:GLN:OE1	2.40	0.54
1:D:1968:ASP:O	1:D:1971:THR:OG1	2.17	0.54
1:D:1603:GLU:O	1:D:1607:LYS:N	2.41	0.53
1:D:2010:SER:O	1:D:2014:GLU:N	2.41	0.53
1:D:17:TYR:O	1:D:220:LYS:N	2.39	0.53
1:C:1194:GLN:NE2	1:C:1234:LYS:O	2.42	0.53
1:C:1053:ARG:NE	1:C:1693:ASN:O	2.43	0.52
1:A:58:LYS:N	1:A:125:LEU:O	2.42	0.52
1:D:656:VAL:HG13	1:D:657:LEU:HD22	1.90	0.52
1:B:827:LYS:O	1:B:831:ALA:N	2.43	0.52
1:D:399:GLN:NE2	1:D:424:GLU:OE2	2.43	0.52
1:D:2329:THR:O	1:D:2333:GLY:N	2.44	0.51
1:B:305:ARG:NH2	1:B:365:SER:O	2.43	0.51
1:A:1385:ILE:O	1:A:1388:THR:OG1	2.15	0.51
1:B:1615:SER:OG	1:B:1687:ARG:NE	2.43	0.51
1:C:153:ASP:OD2	1:C:156:GLY:N	2.42	0.51
1:B:1764:GLY:O	1:B:1883:ASN:ND2	2.44	0.51
1:C:1322:MET:O	1:C:1326:THR:OG1	2.17	0.51
1:D:2507:ILE:O	1:D:2511:LEU:N	2.43	0.51
1:A:1670:GLN:NE2	1:A:1752:GLU:OE1	2.42	0.51
1:C:12:ASP:OD1	1:C:13:ILE:N	2.44	0.50
1:C:730:ARG:NH2	1:C:772:ASP:OD2	2.44	0.50
1:D:1385:ILE:O	1:D:1388:THR:OG1	2.29	0.50
1:A:1787:LYS:NZ	1:A:1791:ASP:OD2	2.44	0.50
1:B:640:SER:O	1:B:643:ILE:N	2.42	0.50
1:B:764:MET:O	1:B:774:ARG:NH2	2.44	0.50
1:B:2150:GLU:OE2	1:B:2304:ARG:NH2	2.44	0.50
1:D:482:PHE:O	1:D:505:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1033:GLU:OE2	1:D:1085:ARG:NH2	2.42	0.50
1:D:1337:ASN:OD1	1:D:1338:ASP:N	2.45	0.50
1:C:2205:GLY:O	1:C:2208:SER:OG	2.25	0.50
1:A:1953:HIS:NE2	1:A:2006:SER:O	2.45	0.50
1:A:2062:ARG:NH1	1:A:2135:GLN:OE1	2.46	0.49
1:C:864:VAL:O	1:C:868:HIS:N	2.46	0.49
1:C:163:PHE:N	1:C:186:ASN:O	2.45	0.49
1:D:1895:GLN:O	1:D:1900:ASN:ND2	2.45	0.49
1:C:1965:ASN:OD1	1:C:2015:ARG:NH2	2.44	0.49
1:B:237:GLY:N	1:B:296:GLY:O	2.46	0.49
1:C:1670:GLN:NE2	1:C:1752:GLU:OE1	2.44	0.49
1:B:663:ASP:OD1	1:B:697:THR:OG1	2.15	0.49
1:A:632:ASP:O	1:A:635:SER:OG	2.23	0.48
1:D:58:LYS:N	1:D:125:LEU:O	2.44	0.48
1:C:1350:LYS:O	1:C:1353:ARG:NH1	2.47	0.48
1:D:1985:ARG:NH2	1:D:1987:ASP:OD2	2.46	0.48
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.47	0.48
1:B:2549:ASP:OD1	1:B:2550:ASN:N	2.47	0.48
1:D:1103:ASP:O	1:D:1107:TYR:N	2.46	0.48
1:B:1350:LYS:O	1:B:1353:ARG:NH1	2.46	0.48
1:D:743:ARG:NH2	1:D:791:GLN:O	2.47	0.48
1:C:141:ALA:N	1:C:147:ALA:O	2.44	0.47
1:B:466:GLN:OE1	1:B:469:ARG:NH2	2.46	0.47
1:D:847:GLU:OE1	1:D:856:LYS:NZ	2.45	0.47
1:D:582:GLN:NE2	1:D:614:GLU:OE2	2.46	0.47
1:D:872:TYR:OH	1:D:973:GLU:O	2.30	0.47
1:A:394:THR:CB	1:A:396:THR:HG1	2.25	0.47
1:A:2536:THR:O	1:A:2545:ARG:N	2.47	0.47
1:D:314:TYR:N	1:D:357:VAL:O	2.45	0.47
1:A:314:TYR:N	1:A:357:VAL:O	2.46	0.47
1:A:2394:ASP:OD1	1:A:2481:ARG:NH2	2.45	0.47
1:B:1229:HIS:NE2	1:B:1260:GLU:OE2	2.48	0.47
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.48	0.47
1:B:2358:VAL:O	1:B:2361:SER:OG	2.16	0.47
1:D:1490:ALA:O	1:D:1494:LYS:N	2.48	0.47
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.48	0.47
1:C:882:LEU:O	1:C:885:THR:OG1	2.26	0.47
1:D:1893:ARG:NH1	1:D:1955:ASN:OD1	2.48	0.46
1:D:2187:LYS:O	1:D:2190:SER:OG	2.20	0.46
1:D:1891:PHE:O	1:D:1895:GLN:NE2	2.48	0.46
1:A:2124:ILE:HD11	1:A:2567:ASN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:OD1	1:B:240:VAL:N	2.47	0.46
1:C:394:THR:CB	1:C:396:THR:HG1	2.28	0.46
1:A:305:ARG:NH2	1:A:365:SER:OG	2.48	0.46
1:B:730:ARG:NH2	1:B:772:ASP:OD2	2.49	0.46
1:B:2058:LEU:O	1:B:2061:SER:OG	2.27	0.46
1:C:507:LYS:NZ	3:C:3002:I3P:O53	2.46	0.46
1:D:180:GLY:O	1:D:220:LYS:NZ	2.49	0.46
1:B:983:LEU:HD21	1:B:1091:THR:HG21	1.98	0.46
1:C:2549:ASP:OD1	1:C:2550:ASN:N	2.47	0.46
1:D:44:ASP:OD1	1:D:45:LEU:N	2.49	0.46
1:D:503:ARG:NH2	1:D:566:ASP:O	2.49	0.46
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.49	0.46
1:D:239:ASP:OD1	1:D:240:VAL:N	2.49	0.46
1:D:1223:GLU:OE1	1:D:1226:ARG:NH2	2.49	0.46
1:D:1965:ASN:OD1	1:D:2015:ARG:NH2	2.49	0.46
1:D:758:ASP:OD1	1:D:759:LEU:N	2.49	0.46
1:A:1280:GLU:OE2	1:A:1284:GLN:NE2	2.49	0.46
1:B:1681:ASP:OD1	1:B:1682:ARG:N	2.49	0.46
1:D:476:LEU:HD23	1:D:479:LEU:HD12	1.98	0.46
1:A:758:ASP:OD1	1:A:759:LEU:N	2.49	0.45
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.49	0.45
1:A:1965:ASN:OD1	1:A:2015:ARG:NH2	2.49	0.45
1:C:838:GLU:O	1:C:842:ASN:OD1	2.34	0.45
1:C:872:TYR:OH	1:C:973:GLU:O	2.32	0.45
1:A:1178:ARG:O	1:A:1182:MET:N	2.50	0.45
1:B:12:ASP:OD1	1:B:13:ILE:N	2.50	0.45
1:B:758:ASP:OD1	1:B:759:LEU:N	2.50	0.45
1:A:1681:ASP:OD1	1:A:1682:ARG:N	2.50	0.45
1:C:714:GLU:O	1:C:718:GLY:N	2.48	0.45
1:B:164:ILE:HG23	1:B:164:ILE:O	2.17	0.45
1:D:164:ILE:HG23	1:D:164:ILE:O	2.17	0.45
1:D:638:CYS:HA	1:D:648:THR:HG21	1.97	0.45
1:D:2124:ILE:HD11	1:D:2567:ASN:O	2.17	0.45
1:A:1043:SER:OG	1:A:1044:MET:N	2.50	0.45
1:D:1735:LYS:NZ	1:D:1739:ASP:OD2	2.50	0.45
1:D:1930:ASN:N	1:D:1933:ASN:OD1	2.48	0.45
1:D:2319:GLU:O	1:D:2323:HIS:ND1	2.48	0.45
1:B:1195:ARG:NH2	1:B:1588:TYR:OH	2.50	0.45
1:A:314:TYR:O	1:A:357:VAL:N	2.50	0.45
1:B:2225:TYR:CE1	1:B:2278:ILE:HG21	2.52	0.45
1:C:164:ILE:HG23	1:C:164:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:SER:O	1:D:486:VAL:HG23	2.18	0.44
1:C:305:ARG:NH2	1:C:365:SER:O	2.51	0.44
1:C:1912:ASP:O	1:C:1916:GLY:N	2.50	0.44
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.50	0.44
1:D:203:ASP:OD1	1:D:204:ASN:N	2.51	0.44
1:A:239:ASP:OD1	1:A:240:VAL:N	2.50	0.44
1:C:1930:ASN:N	1:C:1933:ASN:OD1	2.45	0.44
1:A:1764:GLY:O	1:A:1883:ASN:ND2	2.51	0.44
1:A:2550:ASN:ND2	1:D:2604:ARG:O	2.48	0.44
1:D:1889:GLN:NE2	1:D:1946:GLU:O	2.50	0.44
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.51	0.44
1:D:1930:ASN:OD1	1:D:1931:GLU:N	2.50	0.44
1:A:86:ASP:OD1	1:A:87:VAL:N	2.50	0.43
1:A:165:GLN:O	1:A:184:ILE:N	2.46	0.43
1:A:1365:HIS:CD2	1:A:1413:TYR:HH	2.36	0.43
1:C:2162:ASP:OD1	1:C:2165:GLY:N	2.51	0.43
1:D:886:ARG:NH1	1:D:1047:VAL:O	2.51	0.43
1:C:2598:ASN:OD1	1:C:2599:LEU:N	2.52	0.43
1:A:164:ILE:O	1:A:164:ILE:HG23	2.18	0.43
1:A:563:SER:O	1:A:570:ASN:ND2	2.52	0.43
1:D:86:ASP:OD1	1:D:87:VAL:N	2.52	0.43
1:D:2549:ASP:OD1	1:D:2550:ASN:N	2.48	0.43
1:B:44:ASP:OD1	1:B:45:LEU:N	2.52	0.43
1:D:445:ALA:O	1:D:449:SER:N	2.49	0.43
1:A:255:ASP:OD1	1:A:256:GLU:N	2.51	0.43
1:C:86:ASP:OD1	1:C:87:VAL:N	2.51	0.43
1:C:640:SER:O	1:C:643:ILE:N	2.50	0.43
1:D:192:GLN:NE2	1:D:214:ASN:OD1	2.50	0.43
1:A:466:GLN:OE1	1:A:469:ARG:NH2	2.47	0.42
1:B:2510:ASN:O	1:B:2514:GLY:N	2.52	0.42
1:C:239:ASP:OD1	1:C:240:VAL:N	2.52	0.42
1:D:853:ASN:O	1:D:857:ASN:ND2	2.52	0.42
1:A:1968:ASP:O	1:A:1971:THR:OG1	2.30	0.42
1:C:255:ASP:OD1	1:C:256:GLU:N	2.53	0.42
1:C:772:ASP:OD1	1:C:773:LEU:N	2.52	0.42
1:C:1195:ARG:NH2	1:C:1588:TYR:OH	2.52	0.42
1:D:1987:ASP:OD1	1:D:1988:LEU:N	2.53	0.42
1:D:640:SER:O	1:D:643:ILE:N	2.48	0.42
1:A:772:ASP:OD1	1:A:773:LEU:N	2.52	0.42
1:B:1878:GLN:OE1	1:B:1939:GLN:NE2	2.47	0.42
1:D:2579:ASN:OD1	1:D:2580:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:LYS:O	1:A:831:ALA:N	2.52	0.42
1:B:58:LYS:N	1:B:125:LEU:O	2.48	0.42
1:C:743:ARG:NH1	1:C:787:ASP:O	2.53	0.42
1:D:507:LYS:NZ	3:D:3002:I3P:O53	2.51	0.42
1:B:743:ARG:NH1	1:B:788:ARG:O	2.51	0.42
1:C:44:ASP:OD1	1:C:45:LEU:N	2.52	0.42
1:C:172:SER:OG	1:C:173:ASN:N	2.53	0.41
1:C:1735:LYS:NZ	1:C:1739:ASP:OD2	2.45	0.41
1:C:2552:THR:HG23	1:C:2553:VAL:HG13	2.01	0.41
1:D:19:GLU:OE1	1:D:182:LYS:NZ	2.29	0.41
1:D:314:TYR:O	1:D:357:VAL:N	2.53	0.41
1:A:2367:ARG:NE	1:B:2352:GLU:OE2	2.54	0.41
1:C:1043:SER:OG	1:C:1044:MET:N	2.52	0.41
1:C:2064:ASN:OD1	1:C:2065:LYS:N	2.53	0.41
1:A:2260:SER:OG	1:A:2261:ILE:N	2.54	0.41
1:A:1746:ASN:OD1	1:A:1747:GLU:N	2.53	0.41
1:A:2598:ASN:OD1	1:A:2599:LEU:N	2.52	0.41
1:B:305:ARG:NH2	1:B:365:SER:OG	2.54	0.41
1:B:1912:ASP:O	1:B:1916:GLY:N	2.53	0.41
1:A:1024:ASN:OD1	1:A:1025:LEU:N	2.53	0.41
1:B:1043:SER:OG	1:B:1044:MET:N	2.52	0.41
1:D:2215:ILE:HD12	1:D:2341:TYR:CD2	2.54	0.41
1:A:1350:LYS:O	1:A:1353:ARG:NH1	2.54	0.41
1:B:1054:MET:SD	1:B:1057:ARG:NH2	2.91	0.41
1:A:44:ASP:OD1	1:A:45:LEU:N	2.54	0.41
1:A:1872:PRO:O	1:A:1876:PHE:N	2.47	0.41
1:B:2579:ASN:OD1	1:B:2580:LYS:N	2.54	0.41
1:C:1681:ASP:OD1	1:C:1682:ARG:N	2.54	0.41
1:A:1054:MET:SD	1:A:1057:ARG:NH2	2.94	0.41
1:B:2260:SER:OG	1:B:2261:ILE:N	2.53	0.41
1:B:2598:ASN:OD1	1:B:2599:LEU:N	2.54	0.41
1:D:571:GLN:NE2	1:D:598:LEU:O	2.53	0.41
1:C:2367:ARG:NH2	1:D:2352:GLU:OE2	2.54	0.40
1:A:1411:MET:O	1:A:1415:ASN:ND2	2.54	0.40
1:D:882:LEU:O	1:D:885:THR:OG1	2.29	0.40
1:D:1115:ASP:OD1	1:D:1116:ARG:N	2.54	0.40
1:D:1448:MET:SD	1:D:1469:LEU:HD22	2.62	0.40
1:B:203:ASP:OD1	1:B:204:ASN:N	2.54	0.40
1:C:1107:TYR:OH	1:C:1200:MET:SD	2.61	0.40
1:D:1787:LYS:NZ	1:D:1791:ASP:OD2	2.54	0.40
1:D:1934:VAL:HA	1:D:1937:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:CB	1:B:396:THR:HG1	2.32	0.40
1:C:617:THR:O	1:C:621:LEU:N	2.51	0.40
1:D:801:ARG:NH1	1:D:987:ILE:HG21	2.36	0.40

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 PDB entries followed by that with respect to all EM entries.

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	2144/2671 (80%)	2055 (96%)	89 (4%)	0	100	100
1	B	2144/2671 (80%)	2062 (96%)	82 (4%)	0	100	100
1	C	2144/2671 (80%)	2059 (96%)	85 (4%)	0	100	100
1	D	2152/2671 (81%)	2069 (96%)	83 (4%)	0	100	100
All	All	8584/10684 (80%)	8245 (96%)	339 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	1879/2385 (79%)	1874 (100%)	5 (0%)	91	92
1	B	1879/2385 (79%)	1875 (100%)	4 (0%)	92	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1879/2385 (79%)	1875 (100%)	4 (0%)	92	94
1	D	1927/2385 (81%)	1921 (100%)	6 (0%)	91	92
All	All	7564/9540 (79%)	7545 (100%)	19 (0%)	90	92

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	ARG
1	A	1897	ASN
1	A	1976	ASN
1	A	2289	ASN
1	A	2357	ASN
1	B	390	ARG
1	B	1976	ASN
1	B	2289	ASN
1	B	2357	ASN
1	C	390	ARG
1	C	1976	ASN
1	C	2289	ASN
1	C	2357	ASN
1	D	390	ARG
1	D	1693	ASN
1	D	1902	ASN
1	D	2064	ASN
1	D	2289	ASN
1	D	2357	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	I3P	A	3002	-	24,24,24	1.33	3 (12%)	39,39,39	0.85	0
3	I3P	C	3002	-	24,24,24	1.33	3 (12%)	39,39,39	0.80	2 (5%)
3	I3P	D	3002	-	24,24,24	1.33	3 (12%)	39,39,39	0.87	1 (2%)
3	I3P	B	3002	-	24,24,24	1.33	3 (12%)	39,39,39	0.81	1 (2%)

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
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	C	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	2/15/39/39	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	I3P	P4-O4	3.38	1.65	1.59
3	D	3002	I3P	P1-O1	3.31	1.65	1.59
3	A	3002	I3P	P4-O4	3.29	1.65	1.59
3	B	3002	I3P	P4-O4	3.28	1.65	1.59
3	D	3002	I3P	P4-O4	3.25	1.65	1.59
3	A	3002	I3P	P1-O1	3.22	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	I3P	P1-O1	3.20	1.65	1.59
3	B	3002	I3P	P1-O1	3.20	1.65	1.59
3	A	3002	I3P	P5-O5	3.17	1.65	1.59
3	D	3002	I3P	P5-O5	3.13	1.65	1.59
3	B	3002	I3P	P5-O5	3.12	1.65	1.59
3	C	3002	I3P	P5-O5	3.06	1.64	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3002	I3P	C5-C6-C1	2.12	113.40	109.11
3	B	3002	I3P	P5-O5-C5	-2.04	117.99	123.43
3	C	3002	I3P	P5-O5-C5	-2.02	118.04	123.43
3	C	3002	I3P	P1-O1-C1	-2.01	118.06	123.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3002	I3P	C6-C1-O1-P1
3	B	3002	I3P	C5-O5-P5-O53
3	D	3002	I3P	C5-O5-P5-O53
3	A	3002	I3P	C6-C1-O1-P1
3	B	3002	I3P	C5-O5-P5-O51
3	A	3002	I3P	C4-O4-P4-O43
3	C	3002	I3P	C3-C4-O4-P4

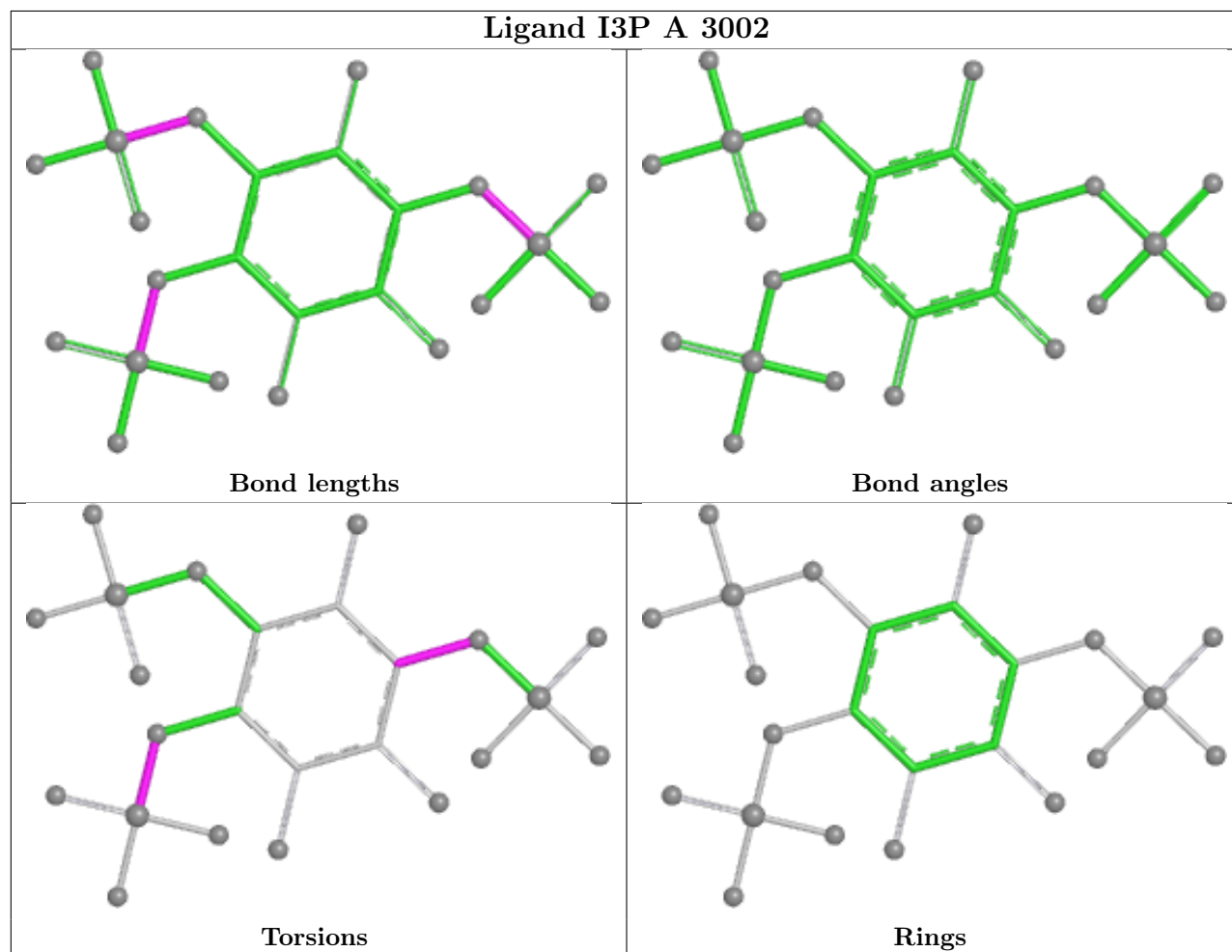
There are no ring outliers.

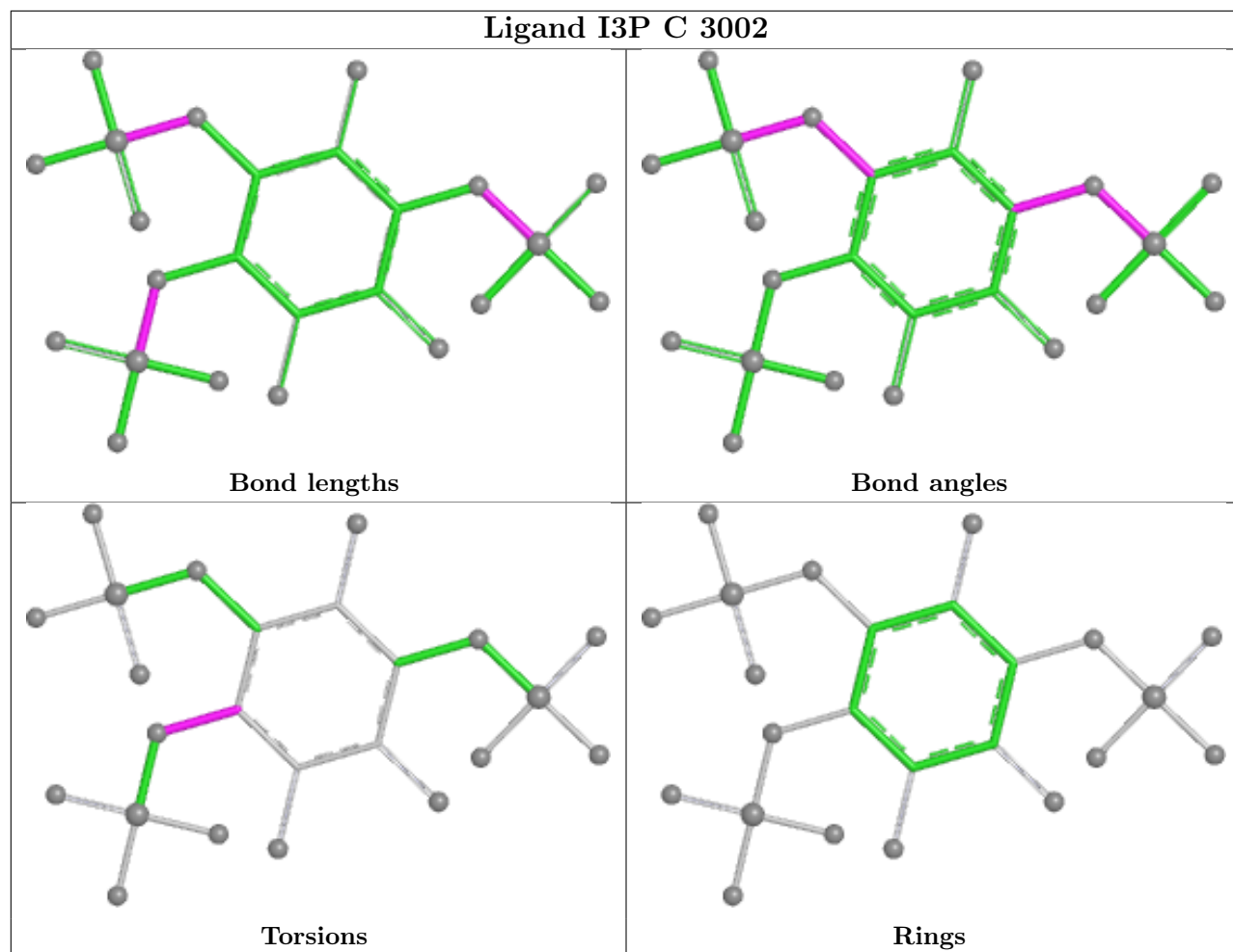
2 monomers are involved in 3 short contacts:

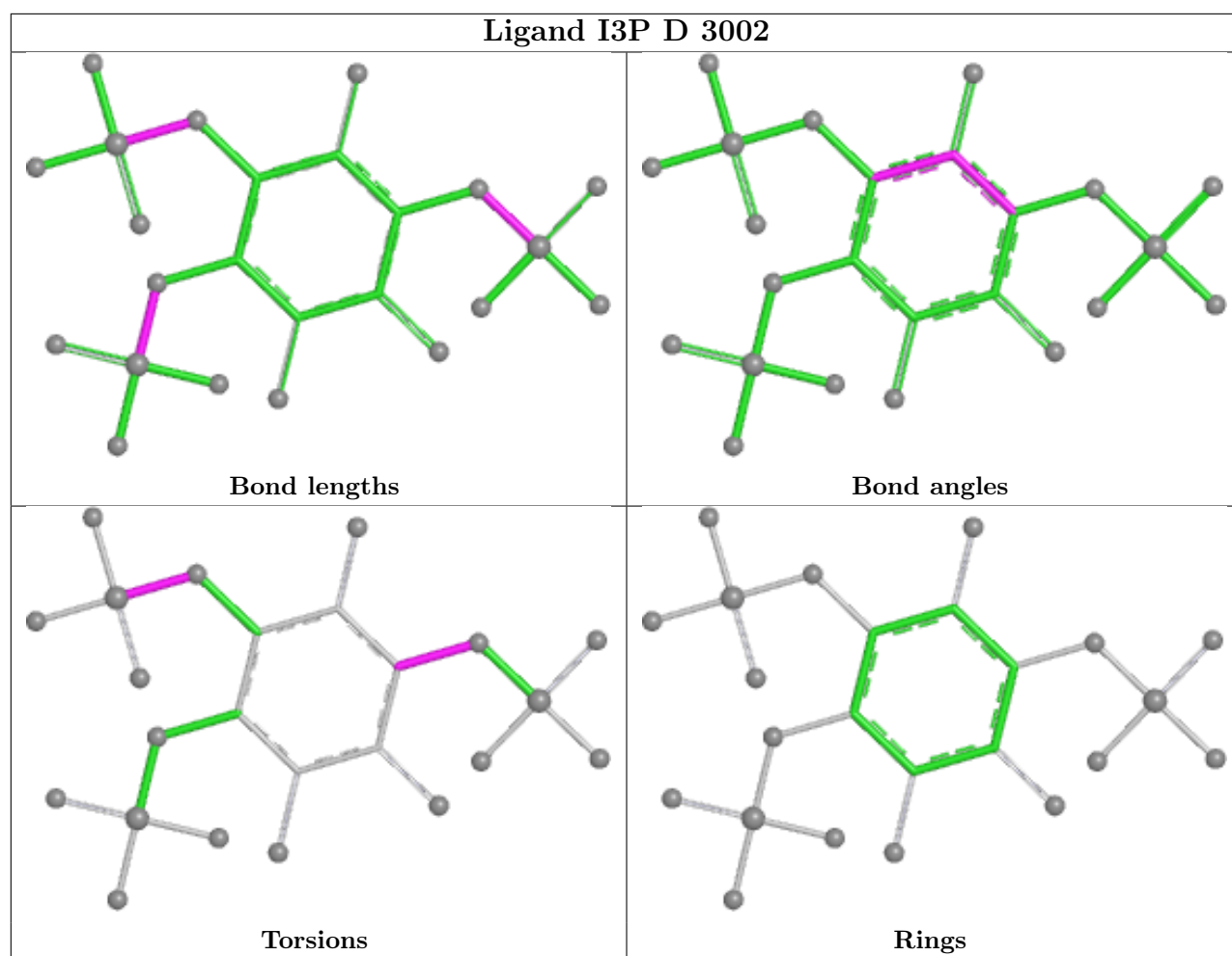
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3002	I3P	2	0
3	D	3002	I3P	1	0

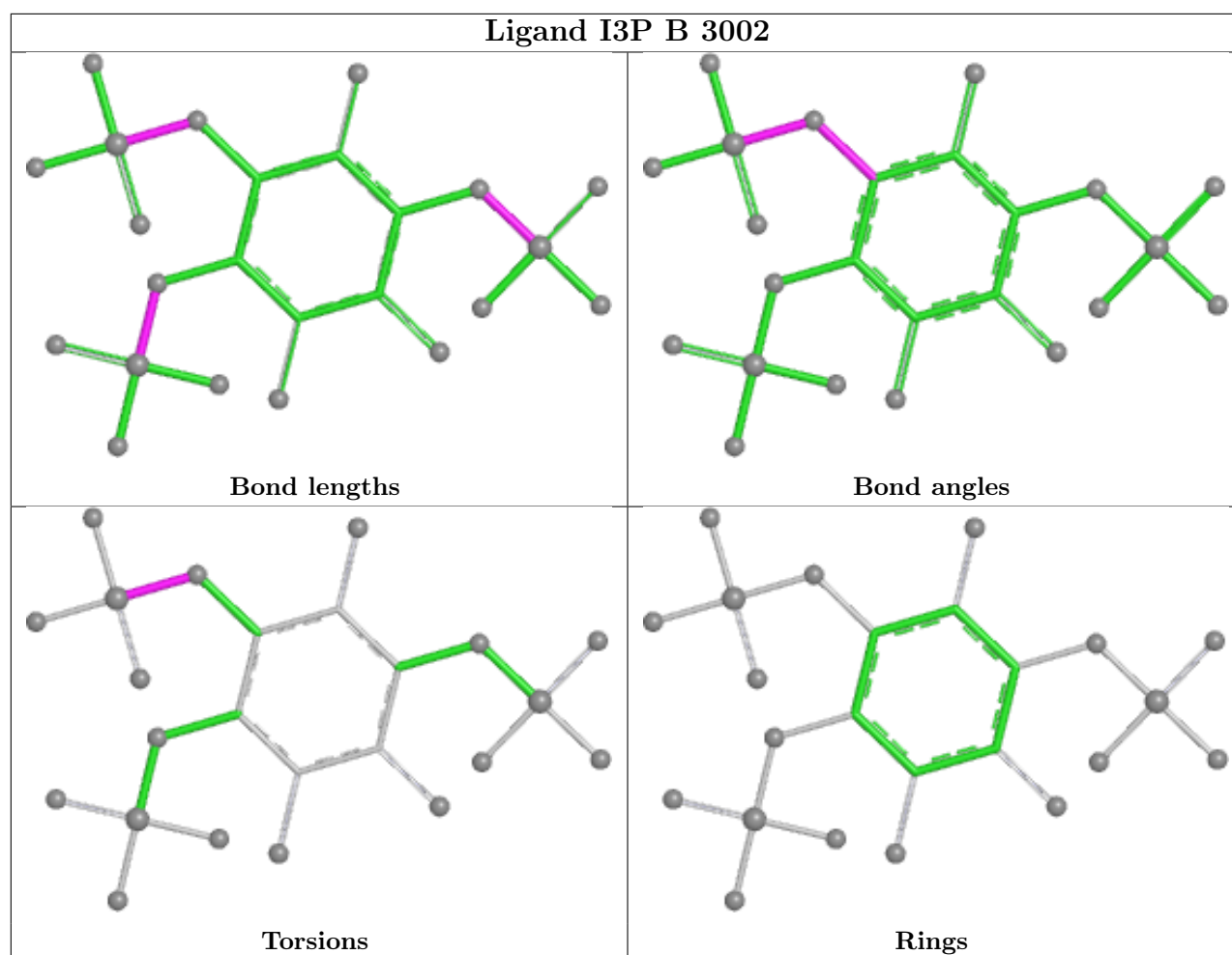
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	5
1	A	5
1	B	5
1	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1552:TRP	C	1587:ASP	N	51.54

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1552:TRP	C	1587:ASP	N	49.80
1	A	1552:TRP	C	1587:ASP	N	49.30
1	B	1552:TRP	C	1587:ASP	N	48.40
1	D	1533:ARG	C	1541:ALA	N	15.42
1	A	1484:ARG	C	1490:ALA	N	15.30
1	C	1484:ARG	C	1490:ALA	N	15.09
1	B	1484:ARG	C	1490:ALA	N	15.07
1	C	1533:ARG	C	1541:ALA	N	14.93
1	A	1533:ARG	C	1541:ALA	N	14.58
1	B	1533:ARG	C	1541:ALA	N	14.30
1	C	1508:GLY	C	1515:ALA	N	8.45
1	A	1508:GLY	C	1515:ALA	N	8.18
1	B	1508:GLY	C	1515:ALA	N	7.81
1	D	2252:TYR	C	2260:SER	N	6.71
1	A	2252:TYR	C	2260:SER	N	6.67
1	C	2252:TYR	C	2260:SER	N	6.25
1	B	2252:TYR	C	2260:SER	N	6.18

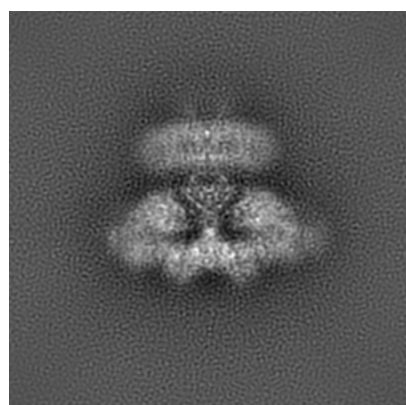
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7983. These allow visual inspection of the internal detail of the map and identification of artifacts.

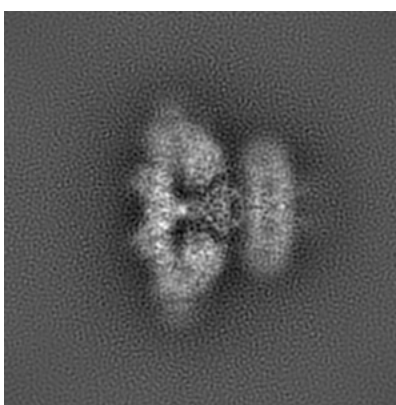
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

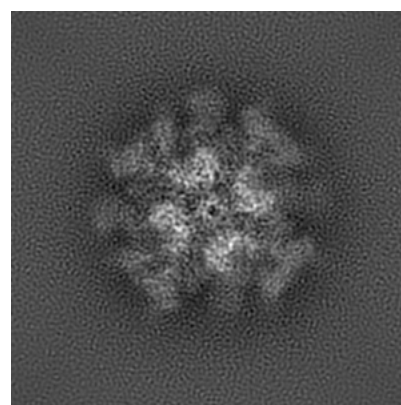
6.1.1 Primary map



X



Y

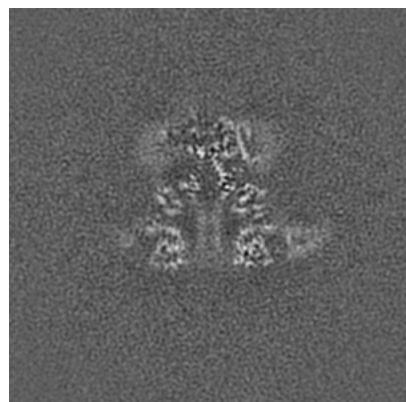


Z

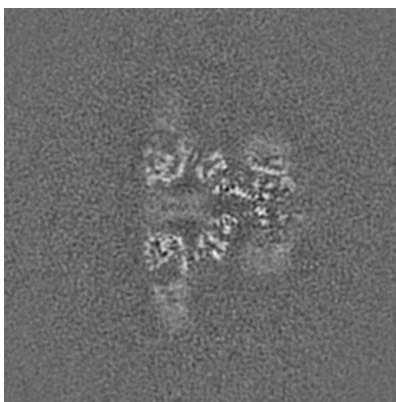
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192

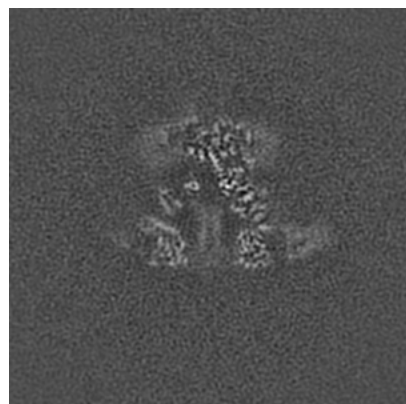


Z Index: 192

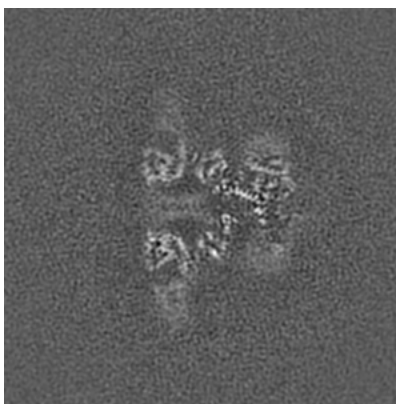
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

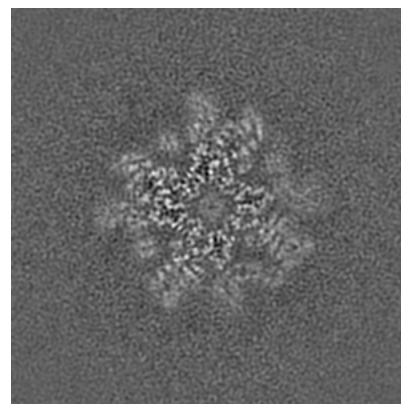
6.3.1 Primary map



X Index: 190



Y Index: 193

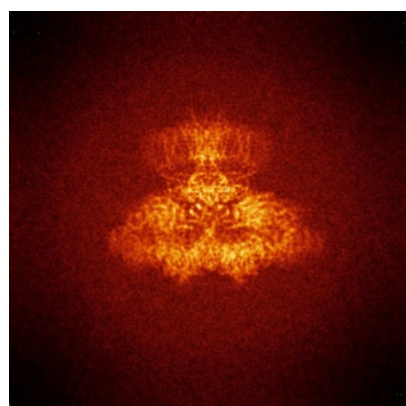


Z Index: 153

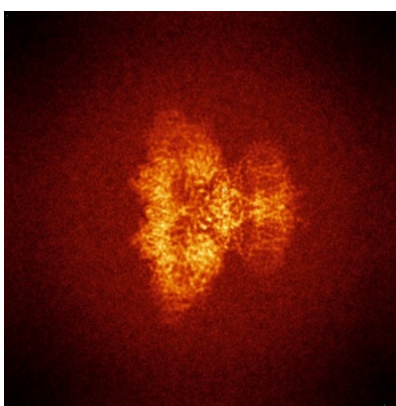
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

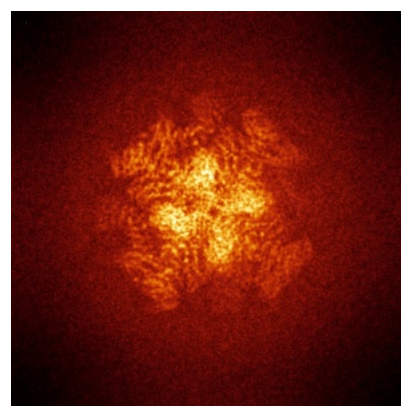
6.4.1 Primary map



X



Y

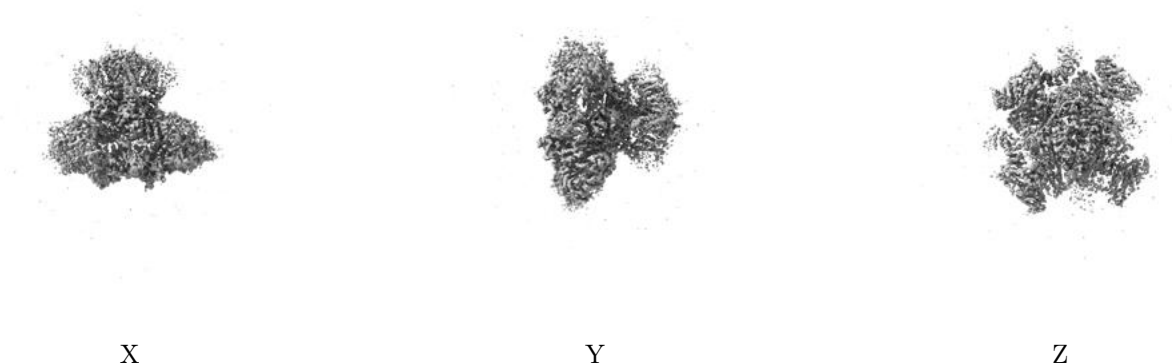


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.93. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

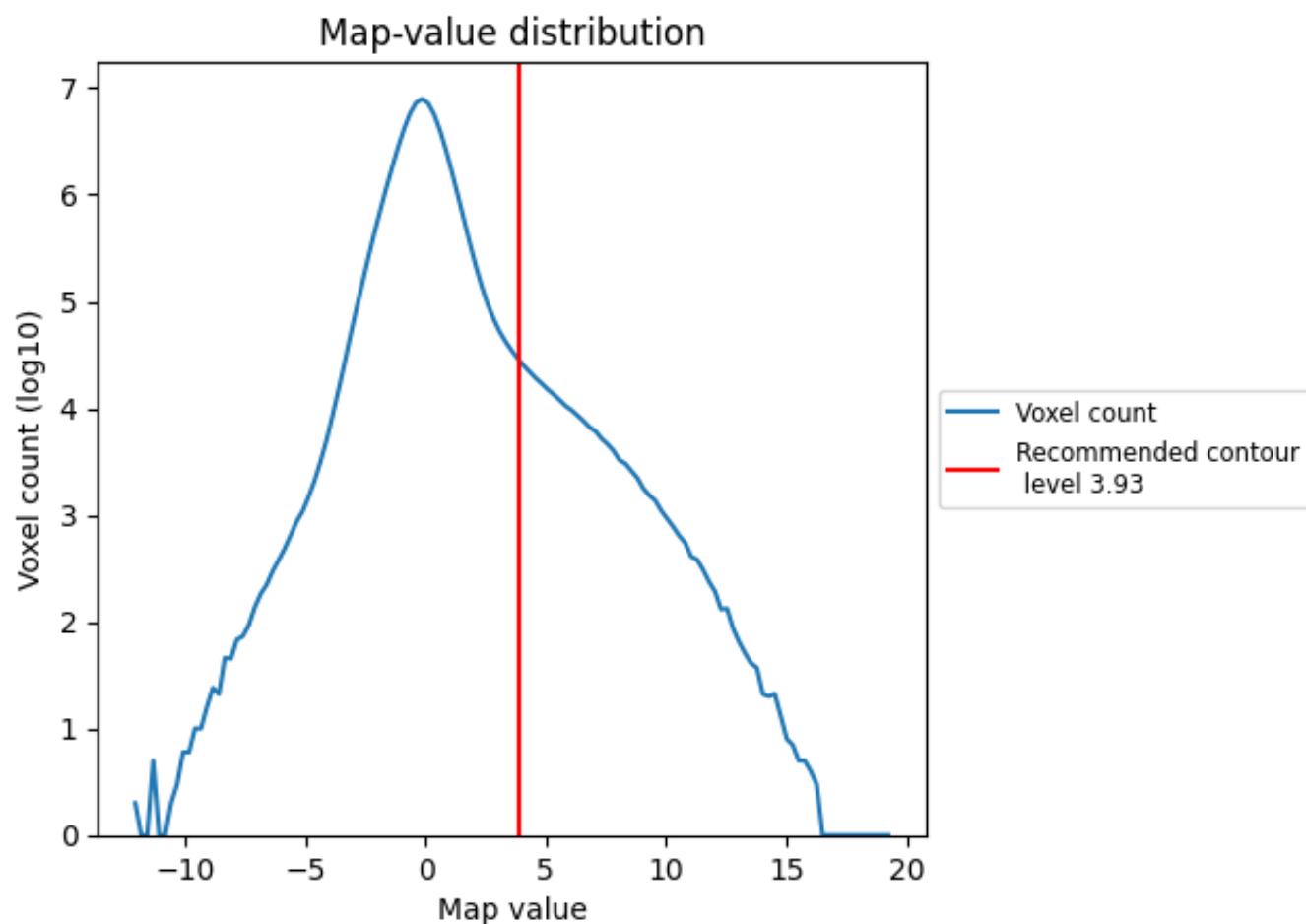
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

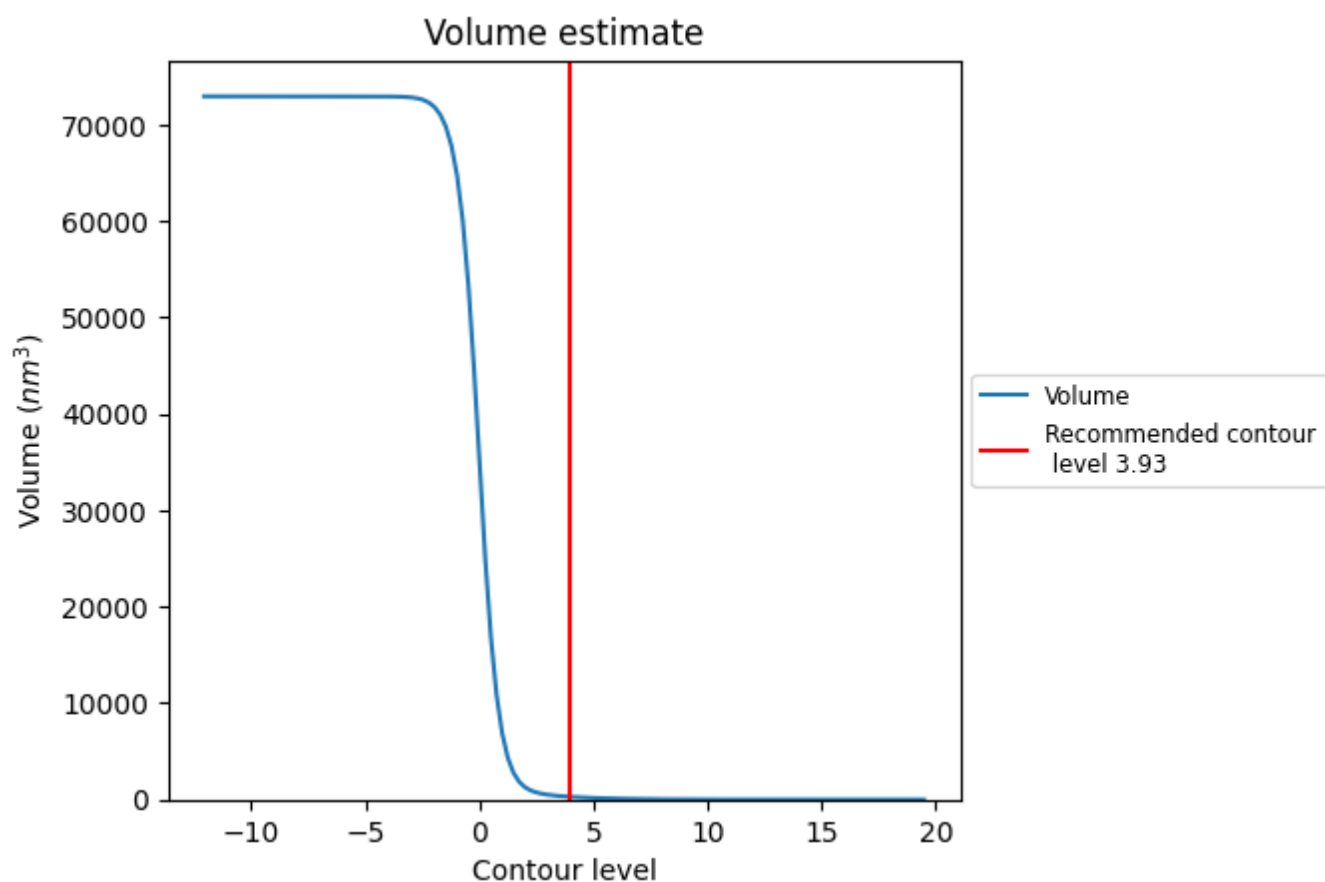
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

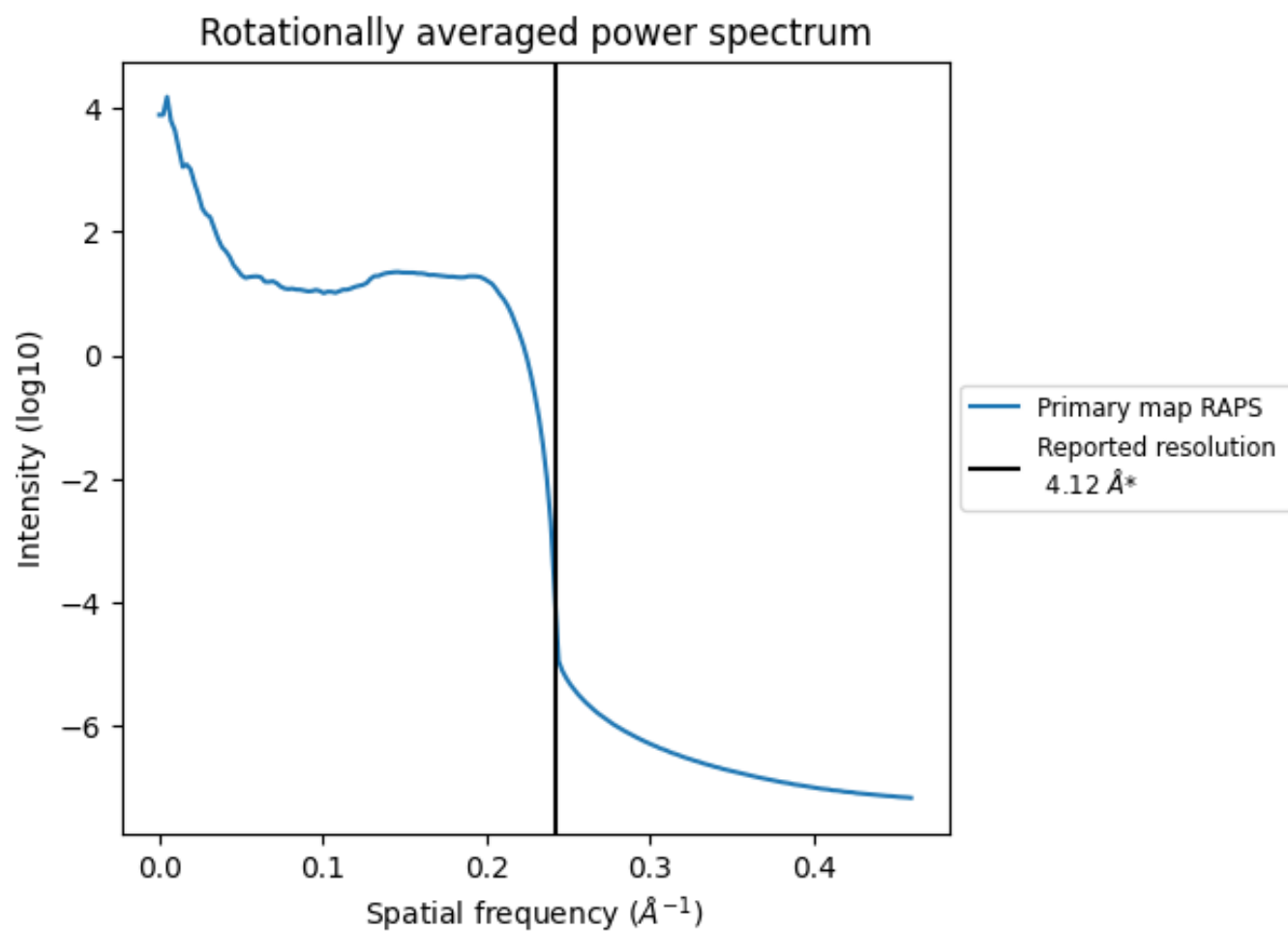
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.243 Å⁻¹

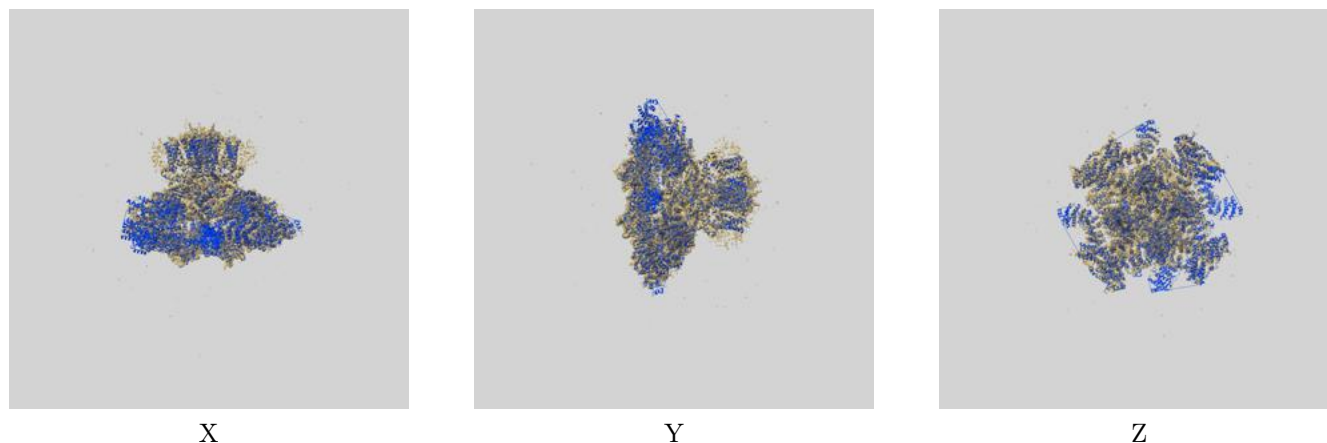
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

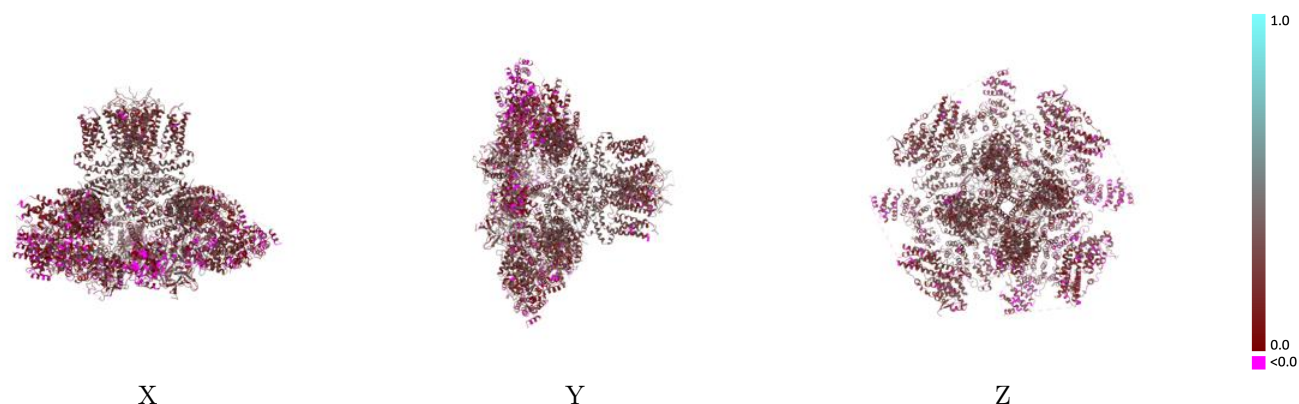
This section contains information regarding the fit between EMDB map EMD-7983 and PDB model 6DQS. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



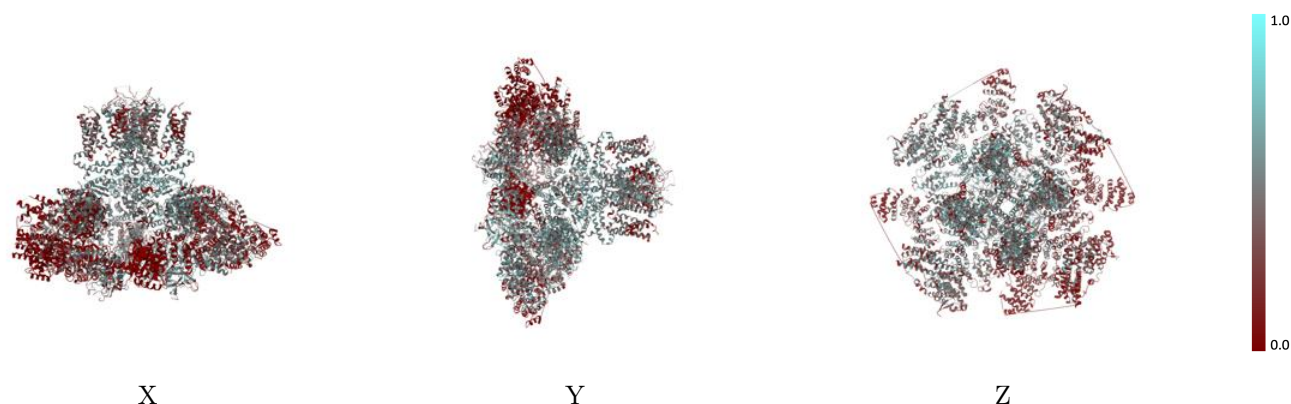
The images above show the 3D surface view of the map at the recommended contour level 3.93 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



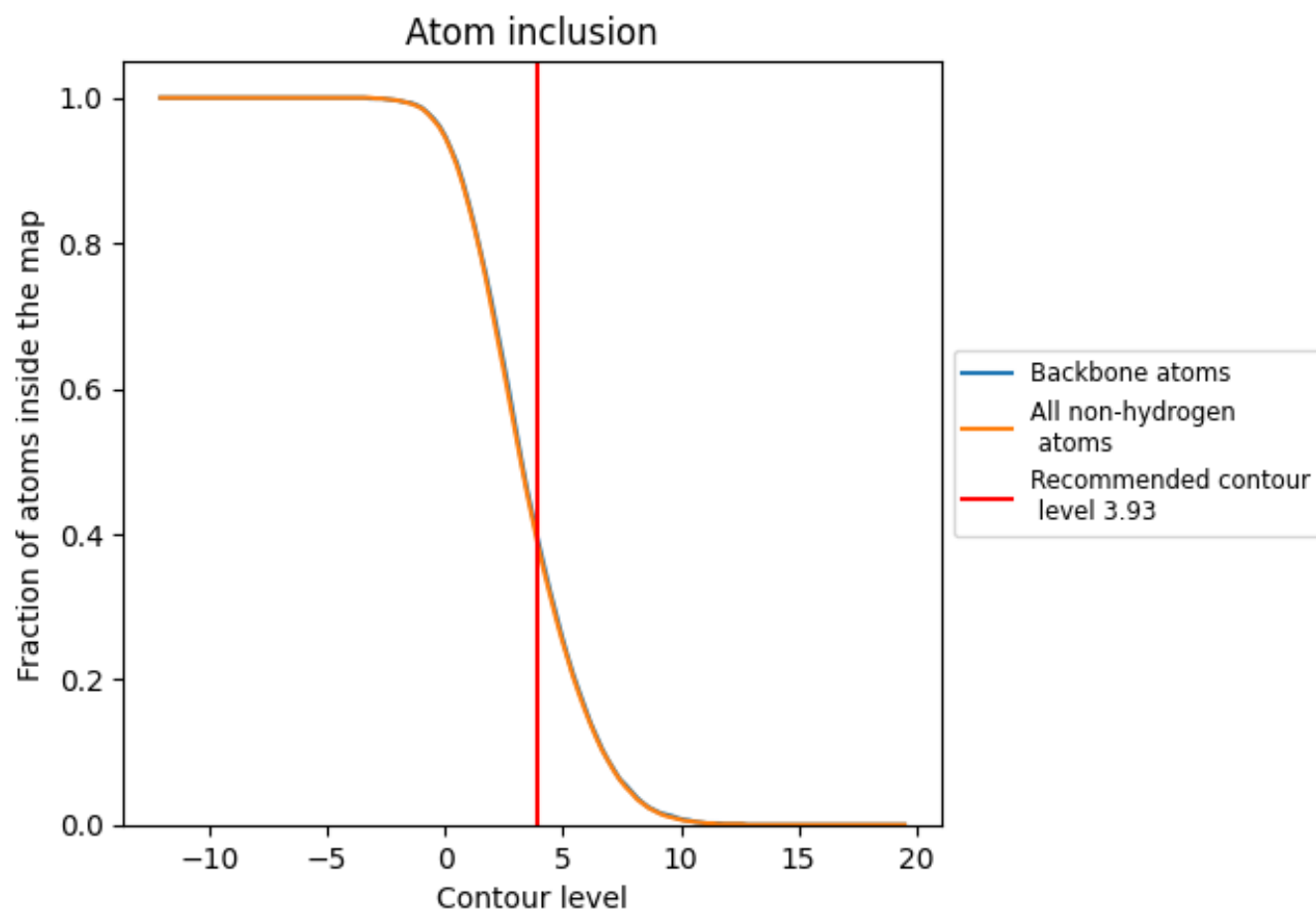
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.93).

9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.93) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3860	<div></div> 0.2360
A	<div></div> 0.3660	<div></div> 0.2260
B	<div></div> 0.4830	<div></div> 0.2670
C	<div></div> 0.4200	<div></div> 0.2460
D	<div></div> 0.3000	<div></div> 0.2050

