



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:18 PM UTC

PDB ID : 8EZJ / pdb_00008ezj
EMDB ID : EMD-28743
Title : Cryo-EM structure of the *S. cerevisiae* Arf-like protein Arl1 bound to the Arf guanine nucleotide exchange factor Gea2
Authors : Duan, H.D.; Li, H.
Deposited on : 2022-11-01
Resolution : 3.30 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:

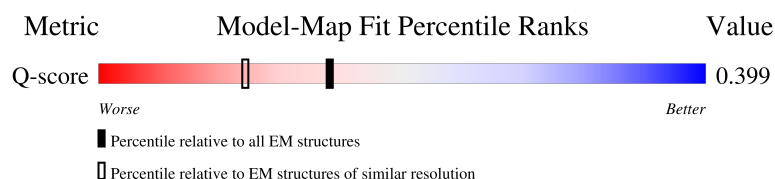
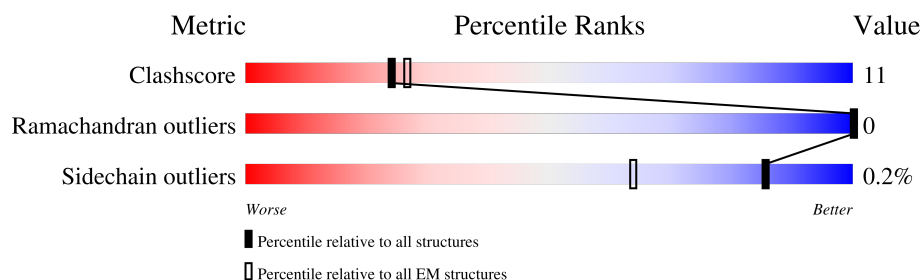
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1483	 66% 21% 13%
1	B	1483	 66% 20% 14%
2	C	183	 63% 27% 10%
2	D	183	 63% 27% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23215 atoms, of which 0 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 ARF guanine-nucleotide exchange factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0
			10319	6622	1680	1980	37		
1	B	1276	Total	C	N	O	S	0	0
			10248	6578	1668	1965	37		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP P39993
A	-22	HIS	-	expression tag	UNP P39993
A	-21	HIS	-	expression tag	UNP P39993
A	-20	HIS	-	expression tag	UNP P39993
A	-19	HIS	-	expression tag	UNP P39993
A	-18	HIS	-	expression tag	UNP P39993
A	-17	HIS	-	expression tag	UNP P39993
A	-16	SER	-	expression tag	UNP P39993
A	-15	SER	-	expression tag	UNP P39993
A	-14	GLY	-	expression tag	UNP P39993
A	-13	VAL	-	expression tag	UNP P39993
A	-12	ASP	-	expression tag	UNP P39993
A	-11	LEU	-	expression tag	UNP P39993
A	-10	GLY	-	expression tag	UNP P39993
A	-9	THR	-	expression tag	UNP P39993
A	-8	GLU	-	expression tag	UNP P39993
A	-7	ASN	-	expression tag	UNP P39993
A	-6	LEU	-	expression tag	UNP P39993
A	-5	TYR	-	expression tag	UNP P39993
A	-4	PHE	-	expression tag	UNP P39993
A	-3	GLN	-	expression tag	UNP P39993
A	-2	SER	-	expression tag	UNP P39993
A	-1	ASN	-	expression tag	UNP P39993
A	0	ALA	-	expression tag	UNP P39993
B	-23	MET	-	initiating methionine	UNP P39993
B	-22	HIS	-	expression tag	UNP P39993

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	HIS	-	expression tag	UNP P39993
B	-20	HIS	-	expression tag	UNP P39993
B	-19	HIS	-	expression tag	UNP P39993
B	-18	HIS	-	expression tag	UNP P39993
B	-17	HIS	-	expression tag	UNP P39993
B	-16	SER	-	expression tag	UNP P39993
B	-15	SER	-	expression tag	UNP P39993
B	-14	GLY	-	expression tag	UNP P39993
B	-13	VAL	-	expression tag	UNP P39993
B	-12	ASP	-	expression tag	UNP P39993
B	-11	LEU	-	expression tag	UNP P39993
B	-10	GLY	-	expression tag	UNP P39993
B	-9	THR	-	expression tag	UNP P39993
B	-8	GLU	-	expression tag	UNP P39993
B	-7	ASN	-	expression tag	UNP P39993
B	-6	LEU	-	expression tag	UNP P39993
B	-5	TYR	-	expression tag	UNP P39993
B	-4	PHE	-	expression tag	UNP P39993
B	-3	GLN	-	expression tag	UNP P39993
B	-2	SER	-	expression tag	UNP P39993
B	-1	ASN	-	expression tag	UNP P39993
B	0	ALA	-	expression tag	UNP P39993

- Molecule 2 is a protein called ADP-ribosylation factor-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	165	Total	C	N	O	S	0	0
			1292	824	211	254	3		
2	D	165	Total	C	N	O	S	0	0
			1292	824	211	254	3		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	72	LEU	GLN	engineered mutation	UNP P38116
C	184	ALA	-	expression tag	UNP P38116
C	185	GLY	-	expression tag	UNP P38116
C	186	GLU	-	expression tag	UNP P38116
C	187	ASN	-	expression tag	UNP P38116
C	188	LEU	-	expression tag	UNP P38116
C	189	TYR	-	expression tag	UNP P38116
C	190	PHE	-	expression tag	UNP P38116

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Chain	Residue	Modelled	Actual	Comment	Reference
C	191	GLN	-	expression tag	UNP P38116
C	192	SER	-	expression tag	UNP P38116
C	193	ALA	-	expression tag	UNP P38116
C	194	GLY	-	expression tag	UNP P38116
C	195	HIS	-	expression tag	UNP P38116
C	196	HIS	-	expression tag	UNP P38116
C	197	HIS	-	expression tag	UNP P38116
C	198	HIS	-	expression tag	UNP P38116
C	199	HIS	-	expression tag	UNP P38116
C	200	HIS	-	expression tag	UNP P38116
D	72	LEU	GLN	engineered mutation	UNP P38116
D	184	ALA	-	expression tag	UNP P38116
D	185	GLY	-	expression tag	UNP P38116
D	186	GLU	-	expression tag	UNP P38116
D	187	ASN	-	expression tag	UNP P38116
D	188	LEU	-	expression tag	UNP P38116
D	189	TYR	-	expression tag	UNP P38116
D	190	PHE	-	expression tag	UNP P38116
D	191	GLN	-	expression tag	UNP P38116
D	192	SER	-	expression tag	UNP P38116
D	193	ALA	-	expression tag	UNP P38116
D	194	GLY	-	expression tag	UNP P38116
D	195	HIS	-	expression tag	UNP P38116
D	196	HIS	-	expression tag	UNP P38116
D	197	HIS	-	expression tag	UNP P38116
D	198	HIS	-	expression tag	UNP P38116
D	199	HIS	-	expression tag	UNP P38116
D	200	HIS	-	expression tag	UNP P38116

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

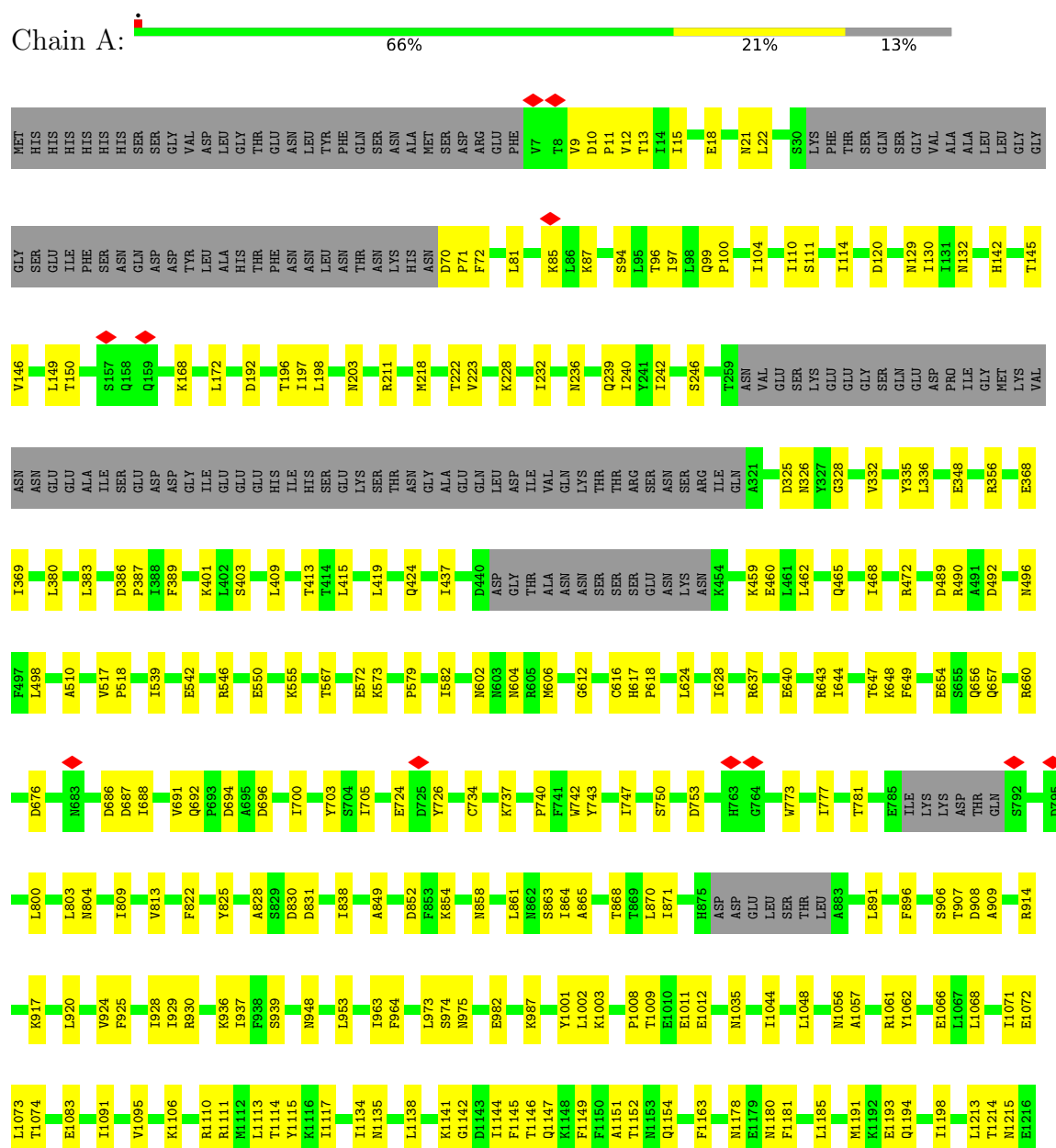


Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: ARF guanine-nucleotide exchange factor 2



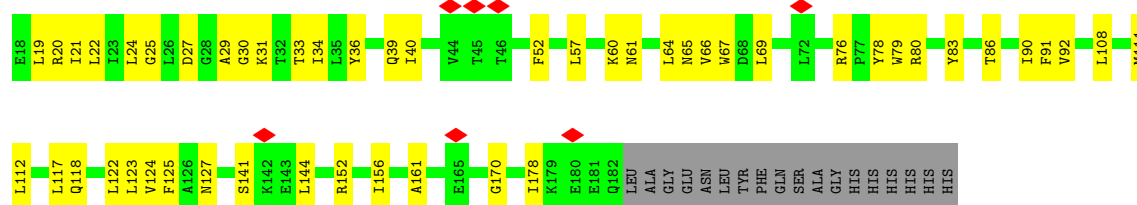
N1217	N1328	ASN
F1218	E1329	ASP
V1221	E1336	VAL
D1226	G1337	ILE
M1231	G1338	GLU
G1232	L1339	ALA
N1236	L1340	THR
H1237	L1342	ALA
H1238	L1355	PRO
E1239	L1359	ILE
I1240	I1362	ASP
E1241	I1362	ASN
Y1242	Y1370	THR
K1243	L1371	ASP
K1244	K1372	ASN
L1245	T1376	LYS
I1246	S1377	PRO
I1252	N1378	GLN
D1253	F1381	LYS
I1269	L1382	LEU
E1277	F1388	SER
D1278	N1389	ASP
R1283	V1392	VAL
K1284	D1396	GLU
N1285	I1397	ASP
E1286	E1398	ASP
H1296	L1401	ASP
Q1297	Q1402	ASP
C1298	D1407	ASP
I1299	I1411	ASP
N1300	N1415	ASP
P1301	G1416	ASP
C1302	S1417	ASP
I1305	SER	SER
V1310	V1311	SER
T1312	T1312	SER
T1316	T1316	SER
L1317	L1317	SER
K1320	K1320	SER
T1323	T1323	SER
P1324	P1324	SER
T1325	T1325	SER
N1326	N1326	SER
E1327	E1327	SER

- Molecule 1: ARF guanine-nucleotide exchange factor 2

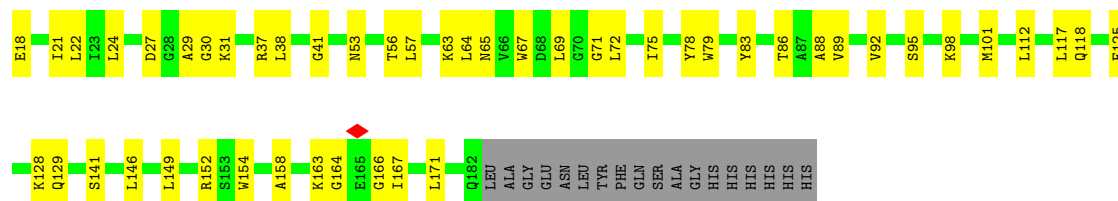
Chain B:  66% 20% 14%

MET	SER	I197	GLY	C734	V529	L409	LEU	N1112	N1236
HIS	GLU	L198	ILE	N735	R541	Q410	SER	L1113	H1237
HIS	ILE	S207	GLU	R746	K560	F412	THR	T1114	W1238
HIS	PHE	E208	GLU	D753	M580	V416	ALA	K1116	E1241
HIS	SER	T217	ILE	I756	L581	I427	PHE	I1117	K1244
HIS	GLN	M218	HIS	V757	E583	L438	GLU	L1118	K1254
SER	ASP	I219	SER	M758	K584	L439	TTR	L1119	E1255
SER	GLY	T222	LYS	P759	I587	D440	GLY	D1122	N1256
VAL	VAL	V223	SER	E766	E597	ASP	P888	A1124	P1257
LEU	LEU	F226	THR	N774	N801	THR	GLY	S1026	I1262
GLY	ASP	S227	ASN	S778	R605	GLY	P894	M1027	S1131
THR	THR	K228	GLY	E785	K608	THR	K895	A1030	L1266
GLU	PHE	L229	ALA	L462	L615	GLY	F896	M1035	L1276
ASN	ASN	K230	GLN	L463	C616	THR	D898	I1044	E1277
ASP	ASN	T231	GLN	L466	H617	THR	T899	L1047	I1290
LYS	ASN	I232	LEU	L488	P618	GLN	V905	L1048	A1295
PRO	ASN	N236	ASP	L498	L624	LYS	S906	E1054	H1296
LYS	ASN	Q239	ILE	L498	D686	ASN	A909	R1055	I1299
SER	ALA	S246	VAL	L498	T690	GLY	I928	M1056	C1302
ASP	MET	L252	GLN	L498	V691	THR	I929	S1060	F1308
VAL	SER	T256	ASN	L498	Q692	LYS	R930	L1061	T1316
GLU	ASP	T259	ARG	L498	D694	THR	N932	Y1062	K1320
ASP	ASP	ASN	ARG	L498	S697	GLY	F938	F1063	N1326
		VAL	ILE	L498	V698	THR	S939	E1064	E1332
		GLU	GLN	L498	L701	THR	K940	I1071	E1336
		SER	GLN	L498	S702	THR	E941	F1072	L1339
		LYS	GLN	L498	Y703	THR	N945	L1073	L1340
		ASP	GLN	L498	S704	THR	I946	T1074	F1341
		PRO	ASP	L498	M721	THR	N950	F1080	L1342
		ILE	ASN	L498	Y726	THR	Y954	C1081	L1343
		GLY	ASN	L498	L522	THR	P961	K1082	T1348
		MET	ASN	L498	V526	THR	D962	L1087	Q1349
		VAL	ASN	L498	T513	THR	L971	I1091	E1350
		ASN	ASN	L498	P518	THR	L973	V1095	D1351
		GLU	GLU	L498	P519	THR	I985	L1098	Q1352
		ALA	GLU	L498	L522	THR	K989	T1101	I1356
		ILE	ALA	L498	V526	THR	S996	K1106	S1357
		SER	ILE	L498		THR		R1107	S1358
		GLY	SER	L498		THR		T1108	
		GLY	GLY	L498		THR		T1109	
		GLY	GLY	L498		THR		R1110	
		GLY	GLY	L498		THR		R1111	

- Molecule 2: ADP-ribosylation factor-like protein 1



- Molecule 2: ADP-ribosylation factor-like protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	712548	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 ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.492	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	423.936, 423.936, 423.936	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/10493	0.33	0/14176
1	B	0.20	0/10419	0.32	0/14075
2	C	0.10	0/1311	0.26	0/1777
2	D	0.14	0/1311	0.31	0/1777
All	All	0.20	0/23534	0.32	0/31805

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	10319	0	10504	224	0
1	B	10248	0	10450	222	0
2	C	1292	0	1312	40	0
2	D	1292	0	1312	38	0
3	C	32	0	12	2	0
3	D	32	0	12	1	0
All	All	23215	0	23602	507	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 11.

All (507) 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)
2:C:24:LEU:O	2:C:31:LYS:HD3	1.69	0.91
1:A:1214:THR:HG22	1:A:1215:ASN:H	1.42	0.83
1:A:1295:ALA:HB1	1:A:1342:LEU:HD22	1.60	0.81
1:B:343:ILE:HD13	1:B:360:LEU:HD23	1.62	0.81
1:B:774:ASN:HA	1:B:778:SER:OG	1.81	0.81
2:C:31:LYS:HE3	2:C:69:LEU:O	1.82	0.80
1:B:1295:ALA:HB1	1:B:1342:LEU:HD22	1.65	0.79
1:B:1348:THR:HB	1:B:1352:GLN:HG3	1.66	0.78
1:A:1213:LEU:HD11	1:A:1218:PHE:CE2	2.19	0.77
2:C:127:ASN:HD21	2:C:161:ALA:HB2	1.50	0.76
1:A:644:ILE:O	1:A:647:THR:HG22	1.86	0.76
2:C:24:LEU:C	2:C:31:LYS:HD3	2.10	0.76
1:B:774:ASN:O	1:B:778:SER:HB2	1.86	0.76
1:A:1214:THR:HG22	1:A:1215:ASN:N	1.99	0.76
1:B:219:ILE:O	1:B:222:THR:HG22	1.85	0.75
2:C:30:GLY:HA2	3:C:301:GTP:H5"	1.68	0.73
1:A:1302:CYS:HB3	1:A:1305:ILE:HB	1.70	0.73
1:B:1339:LEU:O	1:B:1343:LEU:N	2.22	0.71
1:A:643:ARG:NH2	1:A:750:SER:O	2.24	0.71
1:A:1147:GLN:HA	1:A:1191:MET:HE1	1.74	0.70
1:B:581:LEU:HB3	1:B:587:ILE:HD13	1.74	0.69
1:B:198:LEU:HD13	1:B:218:MET:HE2	1.75	0.68
2:C:141:SER:HB3	2:C:156:ILE:HD13	1.76	0.68
1:B:1091:ILE:HG22	1:B:1119:LEU:HD21	1.75	0.68
2:D:149:LEU:HD23	2:D:154:TRP:HB2	1.77	0.67
1:A:15:ILE:HD11	1:A:130:ILE:HG21	1.76	0.67
1:B:1348:THR:HG22	1:B:1349:GLN:N	2.09	0.67
1:B:862:ASN:OD1	1:B:945:ASN:ND2	2.29	0.66
1:B:1082:LYS:NZ	1:B:1122:LEU:O	2.28	0.66
1:B:1276:LEU:HB2	1:B:1290:ILE:HG21	1.78	0.66
1:B:929:ILE:O	1:B:932:ASN:ND2	2.29	0.66
1:B:343:ILE:HG13	1:B:343:ILE:O	1.96	0.66
1:A:409:LEU:HD11	1:A:462:LEU:HD23	1.79	0.65
1:B:343:ILE:CD1	1:B:360:LEU:HD23	2.25	0.65
2:C:108:LEU:HD21	2:C:144:LEU:HD22	1.76	0.65
2:C:117:LEU:O	2:C:152:ARG:NH1	2.29	0.65
1:A:914:ARG:NH1	1:A:1011:GLU:OE1	2.29	0.65
2:D:71:GLY:HA2	2:D:79:TRP:HZ2	1.62	0.64
1:A:838:ILE:HG23	1:A:924:VAL:HG11	1.78	0.64
1:A:1214:THR:CG2	1:A:1215:ASN:H	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:LYS:HG3	1:A:1144:ILE:HG23	1.77	0.64
1:A:1325:THR:HG23	1:A:1328:MET:H	1.62	0.64
1:A:1113:LEU:HD22	1:A:1145:PHE:CZ	2.33	0.64
2:C:91:PHE:HB3	2:C:124:VAL:HG12	1.80	0.64
1:B:1044:ILE:HD12	1:B:1087:LEU:HD21	1.80	0.63
1:A:825:TYR:OH	1:A:838:ILE:HD11	1.98	0.63
1:B:864:ILE:O	1:B:868:THR:HG23	1.98	0.63
1:A:1071:ILE:HD12	1:A:1095:VAL:HG22	1.80	0.63
1:A:539:ILE:HG21	1:A:803:LEU:HD12	1.81	0.63
1:B:1111:ARG:NH2	1:B:1115:TYR:OH	2.28	0.63
1:A:468:ILE:HD13	1:B:20:ILE:HD13	1.79	0.63
1:A:1232:GLY:O	1:A:1236:ASN:ND2	2.32	0.62
1:B:7:VAL:HG12	1:B:8:THR:HG23	1.80	0.62
1:B:488:LEU:O	1:B:605:ARG:NH1	2.31	0.62
1:A:891:LEU:HD13	1:A:906:SER:HB3	1.81	0.62
1:A:618:PRO:HB3	1:A:660:ARG:NH1	2.15	0.62
2:D:117:LEU:O	2:D:152:ARG:NH1	2.29	0.62
1:A:1213:LEU:HD11	1:A:1218:PHE:CD2	2.34	0.62
2:C:60:LYS:NZ	2:C:61:ASN:OD1	2.33	0.62
1:A:11:PRO:HB3	1:A:130:ILE:HG23	1.82	0.62
1:A:336:LEU:HD12	1:A:380:LEU:HD22	1.81	0.62
1:A:838:ILE:CD1	1:A:920:LEU:HB3	2.30	0.62
1:A:838:ILE:HD13	1:A:920:LEU:HB3	1.82	0.61
1:B:1332:GLU:N	1:B:1332:GLU:OE1	2.31	0.61
2:D:18:GLU:N	2:D:63:LYS:O	2.32	0.61
1:A:129:ASN:OD1	1:A:132:ASN:ND2	2.33	0.61
1:B:897:GLU:O	1:B:989:LYS:NZ	2.30	0.61
1:B:734:CYS:SG	1:B:735:ASN:N	2.74	0.61
1:B:757:VAL:HG11	1:B:778:SER:HB3	1.81	0.61
1:B:1332:GLU:HG3	1:B:1380:THR:OG1	1.99	0.61
1:A:825:TYR:CZ	1:A:838:ILE:HD11	2.37	0.60
2:D:95:SER:HB2	2:D:128:LYS:HB2	1.83	0.60
1:A:1299:ILE:HD11	1:A:1342:LEU:HD11	1.83	0.60
1:A:1232:GLY:HA3	1:A:1300:ASN:HD21	1.66	0.60
1:A:424:GLN:OE1	1:A:490:ARG:NH1	2.30	0.59
1:A:930:ARG:O	1:A:1035:ASN:ND2	2.35	0.59
1:B:608:LYS:HG3	1:B:759:PRO:HB2	1.83	0.59
1:B:386:ASP:HB3	1:B:387:PRO:HD3	1.85	0.59
1:B:1172:ARG:NH2	1:B:1210:SER:OG	2.35	0.59
1:B:1071:ILE:HD12	1:B:1095:VAL:HG22	1.83	0.59
1:B:690:THR:HG23	1:B:691:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:ASP:OD1	1:B:899:THR:N	2.36	0.59
1:B:153:ARG:NH1	1:B:256:THR:O	2.36	0.59
1:B:580:MET:HA	1:B:583:GLU:HG2	1.84	0.59
1:A:849:ALA:HA	1:A:937:ILE:HD13	1.85	0.59
1:B:402:LEU:HD21	1:B:457:ILE:CG2	2.33	0.58
1:B:686:ASP:OD1	1:B:746:ARG:NH1	2.36	0.58
1:A:246:SER:HB3	1:A:753:ASP:HB3	1.85	0.58
1:A:386:ASP:HB3	1:A:387:PRO:HD3	1.86	0.58
1:A:870:LEU:HD13	1:A:953:LEU:HD21	1.84	0.58
1:B:906:SER:H	1:B:909:ALA:HB3	1.68	0.58
1:A:401:LYS:NZ	1:A:403:SER:OG	2.37	0.57
1:A:1238:TRP:HH2	1:A:1252:ILE:HG12	1.69	0.57
1:A:492:ASP:O	1:A:496:ASN:ND2	2.37	0.57
1:A:852:ASP:OD2	1:A:936:LYS:NZ	2.37	0.57
1:A:864:ILE:O	1:A:868:THR:HG23	2.05	0.57
1:A:1277:GLU:HG2	1:A:1278:ASP:H	1.69	0.57
1:B:1147:GLN:NE2	1:B:1191:MET:O	2.36	0.57
1:B:693:PRO:HB2	1:B:698:VAL:HG13	1.86	0.57
2:C:25:GLY:O	2:C:31:LYS:NZ	2.33	0.57
1:A:489:ASP:OD1	1:A:602:ASN:ND2	2.34	0.57
1:A:110:ILE:CG2	1:A:114:ILE:HB	2.35	0.56
1:A:676:ASP:O	1:A:692:GLN:NE2	2.33	0.56
1:A:11:PRO:HB3	1:A:130:ILE:HD12	1.86	0.56
1:A:618:PRO:HB3	1:A:660:ARG:HH12	1.71	0.56
2:C:112:LEU:HD11	2:C:122:LEU:HD22	1.87	0.56
1:B:96:THR:O	2:C:78:TYR:OH	2.22	0.56
1:B:774:ASN:O	1:B:778:SER:CB	2.53	0.56
1:A:1245:LEU:HD23	1:A:1252:ILE:HB	1.88	0.56
1:A:10:ASP:N	1:A:10:ASP:OD1	2.38	0.56
1:B:893:GLN:NE2	1:B:902:GLU:OE1	2.39	0.56
1:A:368:GLU:HA	1:B:9:VAL:HG21	1.87	0.55
1:A:468:ILE:HD11	1:B:16:ILE:HG22	1.88	0.55
1:A:510:ALA:HB2	1:A:518:PRO:HG2	1.88	0.55
1:A:825:TYR:CE1	1:A:838:ILE:HD11	2.41	0.55
2:D:21:ILE:HG13	2:D:88:ALA:HB3	1.88	0.55
1:A:489:ASP:HB3	1:A:604:ASN:HB2	1.87	0.55
2:D:29:ALA:HB1	2:D:92:VAL:HG12	1.88	0.55
2:D:125:PHE:HE2	2:D:167:ILE:HA	1.70	0.55
1:A:72:PHE:HB3	1:A:104:ILE:HD11	1.87	0.55
1:B:510:ALA:HB2	1:B:518:PRO:HG2	1.87	0.55
1:B:1343:LEU:HD12	1:B:1356:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:GLN:HG3	2:C:40:ILE:HG23	1.87	0.55
1:A:1072:GLU:OE1	1:A:1115:TYR:OH	2.24	0.55
1:B:198:LEU:HD21	1:B:342:LEU:HD11	1.88	0.55
1:B:492:ASP:OD1	1:B:560:LYS:NZ	2.37	0.55
1:B:597:GLU:OE2	1:B:601:ASN:ND2	2.40	0.55
1:A:222:THR:HG1	1:A:335:TYR:HH	1.51	0.55
1:B:1395:SER:OG	1:B:1399:LYS:NZ	2.40	0.55
1:B:409:LEU:HD11	1:B:462:LEU:HD23	1.89	0.55
1:A:149:LEU:HD21	1:A:172:LEU:HD23	1.89	0.55
1:B:1056:ASN:O	1:B:1060:SER:OG	2.20	0.55
2:C:57:LEU:O	2:C:64:LEU:N	2.34	0.55
1:A:198:LEU:HD13	1:A:218:MET:HE2	1.88	0.54
1:A:800:LEU:O	1:A:804:ASN:ND2	2.33	0.54
1:A:612:GLY:HA2	1:A:649:PHE:CE1	2.43	0.54
1:B:230:LYS:HD2	1:B:370:SER:HA	1.90	0.54
1:B:792:SER:N	1:B:795:ASP:OD2	2.41	0.54
1:A:472:ARG:HD3	1:B:16:ILE:HD12	1.89	0.54
1:A:1151:ALA:HB2	1:A:1193:GLU:HG3	1.90	0.54
1:B:999:ALA:HB1	1:B:1001:TYR:HE1	1.71	0.54
1:A:236:ASN:HB3	1:A:239:GLN:HB3	1.89	0.54
1:A:1253:ASP:OD1	1:A:1253:ASP:N	2.39	0.54
1:A:1388:PHE:HD2	1:A:1401:LEU:HD13	1.72	0.54
1:B:616:CYS:SG	1:B:660:ARG:HB2	2.47	0.54
1:B:1377:SER:OG	1:B:1378:ASN:N	2.37	0.54
1:B:616:CYS:SG	1:B:661:ILE:HG12	2.48	0.54
1:B:928:ILE:HA	1:B:931:ARG:HE	1.72	0.54
1:B:1367:TYR:HE2	1:B:1408:LYS:HG3	1.73	0.54
2:C:92:VAL:HG22	2:C:125:PHE:HB2	1.90	0.54
1:A:242:ILE:HG13	1:A:640:GLU:HB3	1.91	0.53
1:B:946:ILE:O	1:B:950:ILE:HG12	2.08	0.53
1:B:1367:TYR:CD1	1:B:1380:THR:HG21	2.43	0.53
1:A:1342:LEU:HD21	1:A:1355:LEU:HD11	1.90	0.53
1:B:1348:THR:HG21	1:B:1351:ASP:CG	2.33	0.53
2:D:98:LYS:HA	2:D:101:MET:HG2	1.90	0.53
1:A:100:PRO:HD3	2:D:78:TYR:CZ	2.44	0.53
1:A:87:LYS:O	1:B:472:ARG:NH2	2.41	0.53
2:D:112:LEU:O	2:D:118:GLN:NE2	2.42	0.53
2:D:146:LEU:HD13	2:D:154:TRP:HE1	1.74	0.53
1:B:1064:GLU:HB3	1:B:1108:THR:HG21	1.91	0.53
1:B:1011:GLU:OE1	1:B:1011:GLU:N	2.41	0.52
1:A:686:ASP:OD1	1:A:687:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:ALA:O	1:A:917:LYS:NZ	2.30	0.52
1:B:343:ILE:HD13	1:B:360:LEU:CD2	2.38	0.52
1:B:1348:THR:CG2	1:B:1349:GLN:N	2.73	0.52
2:D:89:VAL:HG11	2:D:117:LEU:HD13	1.90	0.52
1:A:18:GLU:HA	1:A:21:ASN:ND2	2.24	0.52
1:B:616:CYS:HB2	1:B:661:ILE:HD11	1.91	0.52
2:C:156:ILE:O	2:C:156:ILE:HG23	2.09	0.52
1:A:1048:LEU:HD11	1:A:1091:ILE:HG13	1.91	0.52
1:B:197:ILE:HG22	1:B:218:MET:HG2	1.92	0.52
1:B:402:LEU:HD21	1:B:457:ILE:HG22	1.91	0.52
1:A:637:ARG:HB3	1:A:743:TYR:CE1	2.45	0.52
1:A:1239:GLU:HA	1:A:1242:TYR:HB3	1.92	0.52
1:B:1266:LEU:HD22	1:B:1308:PHE:HD2	1.75	0.52
2:D:56:THR:HG22	2:D:65:ASN:HD22	1.75	0.52
1:A:1214:THR:CG2	1:A:1215:ASN:N	2.68	0.52
1:A:1389:ASN:HA	1:A:1392:VAL:HB	1.91	0.52
1:B:858:ASN:O	1:B:862:ASN:ND2	2.37	0.52
2:C:36:TYR:HA	2:C:39:GLN:HG2	1.92	0.52
1:A:1152:THR:HG23	1:A:1154:GLN:HB3	1.92	0.51
1:B:149:LEU:HD21	1:B:172:LEU:HD23	1.92	0.51
1:A:437:ILE:O	1:A:459:LYS:NZ	2.43	0.51
1:A:1142:GLY:C	1:A:1144:ILE:H	2.16	0.51
2:C:29:ALA:HB1	2:C:92:VAL:HG12	1.92	0.51
1:A:11:PRO:O	1:A:15:ILE:HG12	2.11	0.51
1:A:1339:LEU:HB3	1:A:1359:ILE:HG23	1.92	0.51
2:C:90:ILE:HD12	2:C:123:LEU:HD22	1.93	0.51
1:A:694:ASP:OD1	1:A:694:ASP:N	2.44	0.51
1:A:1236:ASN:HA	1:A:1239:GLU:HB3	1.92	0.51
1:A:129:ASN:O	1:A:132:ASN:ND2	2.44	0.51
1:B:1123:CYS:SG	1:B:1124:ALA:N	2.84	0.51
2:C:76:ARG:O	2:C:79:TRP:HB2	2.11	0.51
2:C:31:LYS:CE	2:C:69:LEU:O	2.55	0.50
1:B:811:LYS:HD3	1:B:853:PHE:CZ	2.46	0.50
1:B:1340:LEU:HA	1:B:1343:LEU:HB3	1.93	0.50
1:A:1226:ASP:OD1	1:A:1297:GLN:NE2	2.42	0.50
1:A:1317:LEU:O	1:A:1370:TYR:OH	2.28	0.50
1:B:1126:GLN:N	1:B:1171:TYR:OH	2.44	0.50
1:A:12:VAL:HB	1:B:472:ARG:HE	1.76	0.50
1:A:1236:ASN:O	1:A:1240:ILE:HG12	2.11	0.50
2:D:129:GLN:HG3	2:D:158:ALA:HB1	1.93	0.50
1:A:1068:LEU:HD13	1:A:1111:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1131:SER:O	1:B:1135:ASN:ND2	2.25	0.50
1:B:116:SER:OG	1:B:168:LYS:NZ	2.41	0.50
1:B:222:THR:HG23	1:B:223:VAL:N	2.26	0.50
1:A:1284:LYS:HB3	1:A:1327:GLU:OE2	2.12	0.50
1:A:223:VAL:HG22	1:A:369:ILE:HG13	1.94	0.49
1:B:10:ASP:O	1:B:12:VAL:N	2.45	0.49
2:C:65:ASN:OD1	2:C:67:TRP:NE1	2.45	0.49
1:A:861:LEU:HD21	1:A:928:ILE:HG21	1.94	0.49
1:B:1299:ILE:HG21	1:B:1342:LEU:HD11	1.94	0.49
1:A:94:SER:HA	1:A:97:ILE:HD12	1.93	0.49
1:A:734:CYS:O	1:A:737:LYS:HG2	2.12	0.49
1:A:925:PHE:CZ	1:A:929:ILE:HD11	2.46	0.49
1:A:21:ASN:OD1	1:A:22:LEU:N	2.46	0.49
1:B:1178:ASN:HD21	1:B:1180:ASN:HD22	1.59	0.49
1:A:120:ASP:OD1	1:A:168:LYS:NZ	2.36	0.49
1:B:1209:ASP:C	1:B:1211:ASN:H	2.20	0.49
2:D:71:GLY:HA2	2:D:79:TRP:CZ2	2.46	0.49
1:B:1106:LYS:HD2	1:B:1144:ILE:HG22	1.95	0.49
1:B:830:ASP:HB3	1:B:833:ILE:HG22	1.94	0.49
2:D:65:ASN:OD1	2:D:67:TRP:NE1	2.46	0.49
1:A:1396:ASP:OD1	1:A:1396:ASP:N	2.40	0.48
1:B:103:LEU:HD11	2:C:52:PHE:CD1	2.48	0.48
2:C:21:ILE:HB	2:C:66:VAL:HG22	1.94	0.48
2:D:57:LEU:HB2	2:D:64:LEU:HG	1.95	0.48
1:A:1147:GLN:NE2	1:A:1193:GLU:OE2	2.46	0.48
1:B:1150:PHE:O	1:B:1194:GLN:NE2	2.47	0.48
1:B:1415:ASN:OD1	1:B:1416:GLY:N	2.47	0.48
1:A:1338:GLY:O	1:A:1341:PRO:HD2	2.13	0.48
1:B:383:LEU:O	1:B:387:PRO:HD2	2.14	0.48
1:B:1316:THR:HA	1:B:1320:LYS:HG2	1.95	0.48
1:A:1061:ARG:HG3	1:A:1062:TYR:HD2	1.78	0.48
1:B:232:ILE:O	1:B:377:TYR:OH	2.26	0.48
1:B:999:ALA:O	1:B:1001:TYR:N	2.42	0.48
1:B:1071:ILE:HD11	1:B:1098:LEU:HD12	1.95	0.48
1:B:1157:GLU:O	1:B:1161:ARG:HG3	2.14	0.48
1:B:1262:ILE:O	1:B:1266:LEU:HG	2.14	0.48
1:A:415:LEU:HD23	1:A:419:LEU:HD13	1.96	0.48
1:A:686:ASP:OD1	1:A:688:ILE:N	2.36	0.48
1:A:1398:GLU:OE2	1:A:1402:GLN:NE2	2.47	0.48
1:B:954:TYR:CE2	1:B:961:PRO:HB3	2.49	0.48
1:B:999:ALA:HB1	1:B:1001:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ILE:CD1	1:B:360:LEU:CD2	2.91	0.48
1:A:110:ILE:HG22	1:A:111:SER:N	2.28	0.48
1:A:1110:ARG:HD2	1:A:1149:PHE:CD1	2.49	0.48
1:A:1378:ASN:HA	1:A:1381:PHE:HD1	1.79	0.48
1:A:1194:GLN:O	1:A:1198:ILE:HG12	2.14	0.48
2:C:118:GLN:HA	2:C:152:ARG:HH22	1.78	0.48
1:A:654:GLU:OE1	1:A:656:GLN:NE2	2.47	0.47
1:A:1008:PRO:HB3	1:A:1012:GLU:HB2	1.95	0.47
1:B:1348:THR:HG21	1:B:1351:ASP:OD1	2.14	0.47
2:D:22:LEU:HD13	2:D:86:THR:HG23	1.94	0.47
1:A:498:LEU:HD13	1:A:813:VAL:HG11	1.96	0.47
1:B:646:LEU:HD12	1:B:756:ILE:HG21	1.96	0.47
1:B:892:VAL:HG12	1:B:893:GLN:N	2.29	0.47
1:B:928:ILE:HG23	1:B:931:ARG:HH21	1.79	0.47
1:A:222:THR:OG1	1:A:335:TYR:OH	2.22	0.47
1:A:1269:ILE:HG22	1:A:1312:THR:HG21	1.96	0.47
1:B:103:LEU:HD11	2:C:52:PHE:HD1	1.79	0.47
1:B:617:HIS:ND1	1:B:618:PRO:HD2	2.29	0.47
1:A:1002:LEU:HG	1:A:1003:LYS:H	1.79	0.47
1:A:1283:ARG:N	1:A:1286:GLU:OE2	2.44	0.47
1:B:76:PHE:CE1	1:B:100:PRO:HB2	2.50	0.47
1:A:1310:VAL:HG23	1:A:1362:ILE:HD11	1.97	0.47
1:A:1388:PHE:CD2	1:A:1401:LEU:HD13	2.49	0.47
1:B:971:LEU:HD11	1:B:1118:LEU:HD22	1.96	0.47
1:A:325:ASP:O	1:A:326:ASN:C	2.58	0.47
1:A:579:PRO:HA	1:A:582:ILE:HG22	1.96	0.47
1:A:617:HIS:CG	1:A:618:PRO:HD2	2.50	0.47
1:A:830:ASP:OD1	1:A:831:ASP:N	2.47	0.47
1:B:989:LYS:H	1:B:989:LYS:HG2	1.44	0.47
2:D:37:ARG:NH2	2:D:163:LYS:O	2.47	0.47
1:A:100:PRO:HD3	2:D:78:TYR:OH	2.15	0.47
1:B:402:LEU:HD21	1:B:457:ILE:HG21	1.97	0.47
1:B:1348:THR:H	1:B:1352:GLN:NE2	2.13	0.47
2:D:38:LEU:HD22	2:D:171:LEU:HD22	1.96	0.47
2:D:72:LEU:H	2:D:75:ILE:HD11	1.79	0.47
2:D:75:ILE:HA	2:D:78:TYR:HD2	1.78	0.47
1:B:1157:GLU:OE2	1:B:1161:ARG:NH1	2.47	0.47
1:A:460:GLU:OE2	1:B:27:ARG:NH2	2.48	0.47
1:A:1178:ASN:OD1	1:A:1181:PHE:N	2.45	0.47
1:B:1023:ILE:O	1:B:1026:SER:OG	2.25	0.47
2:C:20:ARG:HG2	2:C:86:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:LYS:O	1:A:1110:ARG:HG2	2.14	0.47
1:B:504:LEU:HA	1:B:509:SER:OG	2.15	0.47
2:D:31:LYS:NZ	2:D:69:LEU:O	2.33	0.47
1:A:963:ILE:HG21	1:A:1073:LEU:HD12	1.97	0.46
1:B:1350:GLU:HG2	1:B:1351:ASP:H	1.81	0.46
2:D:56:THR:HB	2:D:63:LYS:HE3	1.95	0.46
1:A:9:VAL:HG21	1:B:368:GLU:HG3	1.95	0.46
1:A:644:ILE:O	1:A:644:ILE:HG22	2.14	0.46
2:C:22:LEU:HD12	2:C:67:TRP:HB2	1.97	0.46
1:B:219:ILE:C	1:B:222:THR:HG22	2.39	0.46
1:B:895:LYS:HG2	1:B:902:GLU:HG2	1.97	0.46
1:B:1348:THR:HG22	1:B:1349:GLN:H	1.77	0.46
1:A:70:ASP:HB3	1:A:71:PRO:HD3	1.98	0.46
1:A:96:THR:O	2:D:78:TYR:OH	2.29	0.46
1:B:228:LYS:HD3	1:B:327:TYR:CE2	2.51	0.46
1:B:666:SER:HB3	1:B:698:VAL:HG23	1.97	0.46
1:B:855:ASP:N	1:B:855:ASP:OD1	2.46	0.46
1:B:1054:GLU:OE1	1:B:1056:ASN:ND2	2.48	0.46
1:B:1109:VAL:HG13	1:B:1145:PHE:HE1	1.81	0.46
2:C:19:LEU:HD13	2:C:178:ILE:HD13	1.98	0.46
1:B:153:ARG:HH12	1:B:256:THR:HB	1.80	0.46
1:B:973:LEU:HB3	1:B:1111:ARG:HH12	1.80	0.46
2:D:53:ASN:OD1	2:D:53:ASN:N	2.48	0.46
1:B:78:GLN:NE2	2:C:80:ARG:HE	2.13	0.46
1:B:932:ASN:O	1:B:1035:ASN:ND2	2.49	0.46
1:A:896:PHE:HA	1:A:987:LYS:O	2.15	0.46
1:B:1098:LEU:O	1:B:1101:THR:OG1	2.29	0.46
2:D:27:ASP:N	2:D:27:ASP:OD1	2.47	0.46
1:B:522:LEU:HD22	1:B:824:ILE:HD13	1.98	0.46
1:A:1106:LYS:HD2	1:A:1110:ARG:HH21	1.81	0.45
1:B:618:PRO:HB3	1:B:660:ARG:NH2	2.30	0.45
1:B:691:VAL:HG12	1:B:693:PRO:HD3	1.97	0.45
2:D:22:LEU:HB3	2:D:24:LEU:HD11	1.97	0.45
1:A:1009:THR:C	1:A:1011:GLU:H	2.23	0.45
1:A:1146:THR:OG1	1:A:1147:GLN:N	2.49	0.45
1:B:498:LEU:HD13	1:B:813:VAL:HG11	1.97	0.45
1:B:1388:PHE:O	1:B:1392:VAL:HG13	2.15	0.45
1:A:705:ILE:HD11	1:A:747:ILE:HD12	1.98	0.45
1:A:838:ILE:CG2	1:A:924:VAL:HG11	2.43	0.45
1:A:197:ILE:HG22	1:A:218:MET:HG2	1.97	0.45
1:A:963:ILE:HG13	1:A:964:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:ASN:O	1:B:735:ASN:ND2	2.48	0.45
1:B:1238:TRP:CD1	1:B:1257:PRO:HD2	2.51	0.45
1:B:1370:TYR:HA	1:B:1373:LEU:HG	1.98	0.45
1:B:236:ASN:OD1	1:B:239:GLN:N	2.44	0.45
1:B:1024:LYS:HE2	1:B:1024:LYS:HB2	1.79	0.45
2:C:24:LEU:O	2:C:31:LYS:CD	2.54	0.45
1:A:1323:ILE:HB	1:A:1324:PRO:HD3	1.99	0.45
1:B:973:LEU:HD21	1:B:1114:THR:HG21	1.98	0.45
1:A:871:ILE:HD13	1:A:948:ASN:HB3	1.98	0.45
1:B:541:ARG:NH1	1:B:852:ASP:OD1	2.49	0.45
1:B:1367:TYR:HD1	1:B:1380:THR:HG21	1.81	0.45
1:B:583:GLU:OE2	1:B:584:LYS:NZ	2.50	0.45
2:C:125:PHE:CZ	2:C:170:GLY:HA3	2.52	0.45
1:A:973:LEU:HB3	1:A:1111:ARG:NH1	2.32	0.45
1:B:246:SER:HB2	1:B:753:ASP:HB3	1.99	0.45
1:A:1323:ILE:O	1:A:1329:GLU:HA	2.17	0.45
1:A:1163:PHE:CE1	1:A:1185:LEU:HD21	2.52	0.44
1:A:724:GLU:C	1:A:726:TYR:H	2.25	0.44
1:A:822:PHE:CZ	1:A:863:SER:HB2	2.53	0.44
2:C:83:TYR:CZ	2:C:111:MET:HG3	2.53	0.44
1:A:777:ILE:O	1:A:781:THR:HG23	2.17	0.44
1:B:962:ASP:OD1	1:B:962:ASP:N	2.51	0.44
1:B:1241:GLU:O	1:B:1244:LYS:HG2	2.18	0.44
1:B:1296:HIS:O	1:B:1299:ILE:HG12	2.17	0.44
1:A:468:ILE:HG21	1:B:17:LYS:HZ3	1.82	0.44
1:A:498:LEU:HD11	1:A:809:ILE:HD11	2.00	0.44
1:B:973:LEU:HB3	1:B:1111:ARG:NH1	2.32	0.44
1:A:142:HIS:O	1:A:145:THR:HG22	2.18	0.44
1:A:228:LYS:O	1:A:232:ILE:HG13	2.18	0.44
1:A:1376:THR:OG1	1:A:1377:SER:N	2.51	0.44
1:A:1407:ASP:O	1:A:1411:ILE:HG12	2.18	0.44
1:B:438:LEU:HB3	1:B:504:LEU:HD11	1.98	0.44
1:A:413:THR:HG21	1:A:465:GLN:O	2.18	0.44
1:A:1411:ILE:O	1:A:1415:ASN:ND2	2.50	0.44
1:B:1348:THR:CG2	1:B:1349:GLN:H	2.30	0.44
1:A:150:THR:HG21	1:A:192:ASP:HB3	1.99	0.44
1:A:1277:GLU:OE1	1:A:1320:LYS:NZ	2.45	0.44
1:B:472:ARG:HA	1:B:472:ARG:HD2	1.76	0.44
1:B:1061:ARG:HG3	1:B:1062:TYR:HD2	1.82	0.44
1:A:110:ILE:HG21	1:A:114:ILE:HB	2.00	0.44
1:A:242:ILE:HD11	1:A:644:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1027:ASN:OD1	1:B:1030:ALA:HB3	2.18	0.44
1:A:861:LEU:HD23	1:A:861:LEU:HA	1.80	0.44
1:A:1001:TYR:HB2	1:A:1002:LEU:H	1.61	0.44
1:A:1336:GLU:HA	1:A:1340:LEU:HB3	1.99	0.44
1:B:207:SER:OG	1:B:208:GLU:N	2.51	0.44
1:B:509:SER:O	1:B:513:THR:OG1	2.22	0.44
1:B:1167:GLU:OE2	1:B:1172:ARG:NH1	2.50	0.44
1:B:615:LEU:O	1:B:624:LEU:HB2	2.18	0.43
1:B:1336:GLU:O	1:B:1340:LEU:HB3	2.18	0.43
1:A:974:SER:O	1:A:975:ASN:HB2	2.17	0.43
1:A:1372:LYS:HG2	1:A:1411:ILE:HD12	2.00	0.43
1:B:474:PRO:C	1:B:476:PHE:H	2.26	0.43
1:A:907:THR:HG23	1:A:908:ASP:N	2.33	0.43
1:B:1375:LYS:HG3	1:B:1376:THR:HG23	2.00	0.43
2:C:141:SER:HB3	2:C:156:ILE:CD1	2.45	0.43
1:A:1231:MET:SD	1:A:1231:MET:N	2.91	0.43
1:B:1113:LEU:HD22	1:B:1145:PHE:CE2	2.53	0.43
2:C:33:THR:HG23	3:C:301:GTP:H5'	2.00	0.43
1:A:1243:LYS:HA	1:A:1246:THR:OG1	2.18	0.43
1:A:1044:ILE:HG23	1:A:1074:THR:OG1	2.19	0.43
1:B:638:VAL:HG22	1:B:669:TYR:CE2	2.53	0.43
1:B:1254:LYS:HG3	1:B:1255:GLU:O	2.19	0.43
2:D:141:SER:HA	2:D:146:LEU:HD12	2.01	0.43
1:A:1142:GLY:C	1:A:1144:ILE:N	2.76	0.43
1:B:694:ASP:N	1:B:697:SER:OG	2.52	0.43
2:C:124:VAL:HG23	2:C:156:ILE:HA	2.00	0.43
1:A:142:HIS:O	1:A:146:VAL:HG23	2.18	0.43
1:A:203:ASN:O	1:A:211:ARG:NH1	2.44	0.43
1:A:517:VAL:HB	1:A:518:PRO:HD3	2.00	0.42
1:A:550:GLU:HB2	1:A:555:LYS:HE3	2.00	0.42
1:B:463:ILE:HD12	1:B:463:ILE:HA	1.83	0.42
1:A:891:LEU:O	1:A:982:GLU:HB2	2.18	0.42
1:A:100:PRO:O	1:A:104:ILE:HG12	2.20	0.42
1:A:110:ILE:CG2	1:A:111:SER:N	2.82	0.42
1:A:572:GLU:HG3	1:A:573:LYS:HG2	2.02	0.42
1:B:219:ILE:O	1:B:223:VAL:HG23	2.19	0.42
1:B:1165:LEU:HD11	1:B:1171:TYR:HD2	1.84	0.42
1:A:1062:TYR:HD1	1:A:1066:GLU:HG3	1.84	0.42
1:B:174:ARG:HB2	1:B:217:THR:HG23	2.00	0.42
1:B:526:VAL:HA	1:B:529:VAL:HG12	2.00	0.42
1:B:1405:ILE:HG13	1:B:1406:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:GLN:HA	2:D:152:ARG:NH2	2.35	0.42
1:B:1117:ILE:HD12	1:B:1117:ILE:HA	1.85	0.42
1:A:348:GLU:HA	1:A:356:ARG:NH1	2.35	0.42
1:A:1378:ASN:HA	1:A:1381:PHE:CD1	2.55	0.42
1:B:412:PHE:O	1:B:416:VAL:HG23	2.20	0.42
1:A:1336:GLU:O	1:A:1341:PRO:HD3	2.20	0.42
1:B:938:PHE:HD2	1:B:942:LEU:HD23	1.84	0.42
1:B:392:ILE:HD11	1:B:411:LEU:HD23	2.02	0.42
1:B:439:LEU:HD22	1:B:503:LYS:HD2	2.02	0.42
2:D:164:GLY:O	2:D:166:GLY:N	2.53	0.42
1:A:854:LYS:HG2	1:A:858:ASN:HD21	1.83	0.42
1:A:953:LEU:HD13	1:A:953:LEU:HA	1.92	0.42
1:B:16:ILE:O	1:B:20:ILE:HG23	2.20	0.42
1:B:139:ILE:HG12	1:B:184:LEU:HD23	2.01	0.42
1:B:954:TYR:HE2	1:B:961:PRO:HB3	1.85	0.42
1:B:1150:PHE:HB3	1:B:1194:GLN:HE22	1.85	0.42
1:A:936:LYS:HE3	1:A:936:LYS:HB3	1.89	0.41
1:B:222:THR:CG2	1:B:223:VAL:N	2.83	0.41
1:B:226:PHE:O	1:B:229:LEU:HB3	2.20	0.41
1:B:893:GLN:O	1:B:985:ILE:HG22	2.19	0.41
2:C:30:GLY:O	2:C:34:ILE:HG12	2.20	0.41
1:A:99:GLN:HB3	2:D:78:TYR:CE2	2.56	0.41
1:B:1114:THR:O	1:B:1117:ILE:HG22	2.20	0.41
1:B:1213:LEU:HD23	1:B:1213:LEU:HA	1.92	0.41
1:A:150:THR:HG23	1:A:196:THR:OG1	2.21	0.41
1:A:696:ASP:O	1:A:700:ILE:HG12	2.20	0.41
1:A:906:SER:H	1:A:909:ALA:HB3	1.86	0.41
1:B:1048:LEU:HA	1:B:1048:LEU:HD23	1.79	0.41
1:B:1350:GLU:CD	1:B:1350:GLU:H	2.29	0.41
1:B:1388:PHE:O	1:B:1392:VAL:N	2.54	0.41
2:D:24:LEU:HA	2:D:31:LYS:HZ1	1.85	0.41
1:B:616:CYS:HG	1:B:661:ILE:HG12	1.84	0.41
1:B:1236:ASN:HB2	1:B:1302:CYS:HA	2.02	0.41
2:D:30:GLY:N	3:D:301:GTP:O2B	2.53	0.41
1:A:336:LEU:HB3	1:A:383:LEU:HD13	2.02	0.41
1:A:539:ILE:HG13	1:A:803:LEU:HD11	2.03	0.41
1:A:656:GLN:H	1:A:656:GLN:CD	2.28	0.41
1:A:858:ASN:CG	1:A:939:SER:HB3	2.45	0.41
1:A:1141:LYS:HD3	1:A:1141:LYS:HA	1.93	0.41
1:B:124:LYS:HA	1:B:127:THR:HG22	2.01	0.41
1:B:1228:ILE:O	1:B:1231:MET:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1326:ASN:C	1:B:1328:MET:H	2.28	0.41
2:D:37:ARG:HD2	2:D:41:GLY:HA2	2.03	0.41
1:A:81:LEU:O	1:A:85:LYS:HG2	2.21	0.41
1:A:142:HIS:HA	1:A:145:THR:HG22	2.03	0.41
1:A:1135:ASN:OD1	1:A:1180:ASN:ND2	2.54	0.41
1:A:1217:ASN:O	1:A:1221:VAL:HG22	2.20	0.41
1:A:1232:GLY:HA3	1:A:1300:ASN:ND2	2.33	0.41
1:A:10:ASP:O	1:A:13:THR:HG22	2.21	0.41
1:A:567:THR:HG22	1:A:606:MET:HE1	2.02	0.41
1:B:198:LEU:HD23	1:B:252:LEU:HD13	2.03	0.41
1:B:219:ILE:HD13	1:B:362:LEU:HD23	2.03	0.41
1:B:416:VAL:HG13	1:B:427:ILE:HD13	2.02	0.41
1:B:940:LYS:HE3	1:B:940:LYS:HB3	1.95	0.41
2:C:27:ASP:OD1	2:C:27:ASP:N	2.52	0.41
1:A:1083:GLU:CD	1:A:1083:GLU:H	2.28	0.41
1:B:1150:PHE:HB3	1:B:1194:GLN:NE2	2.36	0.41
1:A:328:GLY:O	1:A:332:VAL:HG23	2.21	0.41
1:A:386:ASP:OD1	1:A:773:TRP:NE1	2.51	0.41
1:A:616:CYS:SG	1:A:657:GLN:HA	2.61	0.41
1:A:644:ILE:O	1:A:644:ILE:CG2	2.69	0.41
1:B:518:PRO:HB2	1:B:519:PRO:HD3	2.03	0.41
1:B:701:LEU:O	1:B:704:SER:OG	2.29	0.41
1:B:766:GLU:H	1:B:766:GLU:CD	2.28	0.41
1:B:811:LYS:HD3	1:B:853:PHE:CE1	2.56	0.41
1:B:1011:GLU:OE2	1:B:1012:GLU:HG3	2.21	0.41
1:B:1044:ILE:HG23	1:B:1074:THR:HG23	2.03	0.41
1:B:1047:LEU:HD21	1:B:1073:LEU:HB3	2.03	0.41
1:B:1367:TYR:CD1	1:B:1380:THR:CG2	3.04	0.41
1:B:1404:LEU:HA	1:B:1407:ASP:OD2	2.21	0.41
1:A:647:THR:HG23	1:A:648:LYS:N	2.36	0.41
1:A:1316:THR:O	1:A:1320:LYS:HB2	2.21	0.41
1:B:721:MET:HE2	1:B:726:TYR:HA	2.03	0.41
1:B:1166:THR:HG21	1:B:1201:TYR:OH	2.21	0.41
1:A:240:ILE:H	1:A:240:ILE:HG13	1.67	0.40
1:A:1056:ASN:OD1	1:A:1057:ALA:N	2.54	0.40
1:A:1114:THR:O	1:A:1117:ILE:HG22	2.21	0.40
1:A:1134:ILE:HD13	1:A:1138:LEU:HD12	2.02	0.40
1:B:1358:SER:O	1:B:1362:ILE:HG12	2.20	0.40
1:A:624:LEU:O	1:A:628:ILE:HG12	2.21	0.40
1:A:803:LEU:HD23	1:A:803:LEU:HA	1.77	0.40
1:A:865:ALA:HA	1:A:868:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:ASN:C	1:A:1180:ASN:H	2.30	0.40
1:A:1378:ASN:O	1:A:1382:LEU:HG	2.22	0.40
1:B:1087:LEU:O	1:B:1091:ILE:HD13	2.22	0.40
1:A:691:VAL:HG11	1:A:743:TYR:HD2	1.87	0.40
1:B:70:ASP:HB3	1:B:71:PRO:HD3	2.02	0.40
1:B:891:LEU:HD12	1:B:905:VAL:O	2.22	0.40
1:B:903:ILE:HG23	1:B:1020:MET:HE2	2.03	0.40
1:B:1277:GLU:HG3	1:B:1320:LYS:NZ	2.36	0.40
2:C:24:LEU:HD22	2:C:111:MET:HE2	2.04	0.40
1:A:336:LEU:HD23	1:A:336:LEU:HA	1.84	0.40
1:A:542:GLU:O	1:A:546:ARG:HG3	2.22	0.40
1:A:740:PRO:HB2	1:A:742:TRP:CD1	2.56	0.40
1:A:1371:LEU:HD13	1:A:1381:PHE:HZ	1.86	0.40
1:B:1185:LEU:HA	1:B:1188:VAL:HG12	2.03	0.40
1:B:1348:THR:HG21	1:B:1351:ASP:OD2	2.22	0.40
2:D:83:TYR:CD1	2:D:117:LEU:HD11	2.56	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	1273/1483 (86%)	1151 (90%)	122 (10%)	0	100	100
1	B	1264/1483 (85%)	1161 (92%)	103 (8%)	0	100	100
2	C	163/183 (89%)	151 (93%)	12 (7%)	0	100	100
2	D	163/183 (89%)	155 (95%)	8 (5%)	0	100	100
All	All	2863/3332 (86%)	2618 (91%)	245 (9%)	0	100	100

There are no Ramachandran outliers to report.

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 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	1191/1367 (87%)	1189 (100%)	2 (0%)	87	88
1	B	1184/1367 (87%)	1180 (100%)	4 (0%)	86	86
2	C	142/156 (91%)	142 (100%)	0	100	100
2	D	142/156 (91%)	142 (100%)	0	100	100
All	All	2659/3046 (87%)	2653 (100%)	6 (0%)	85	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	PHE
1	A	703	TYR
1	B	171	PHE
1	B	389	PHE
1	B	703	TYR
1	B	1080	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	132	ASN
1	A	212	ASN
1	A	487	ASN
1	A	617	HIS
1	A	672	ASN
1	A	683	ASN
1	A	858	ASN
1	A	1180	ASN
1	A	1236	ASN
1	A	1256	ASN
1	B	729	ASN
1	B	765	ASN

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Mol	Chain	Res	Type
1	B	823	ASN
1	B	932	ASN
1	B	968	GLN
1	B	1180	ASN
1	B	1285	ASN
1	B	1297	GLN
1	B	1369	HIS
1	B	1389	ASN
2	D	131	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	GTP	D	301	-	33,34,34	0.91	1 (3%)	50,54,54	1.62	9 (18%)
3	GTP	C	301	-	33,34,34	0.95	1 (3%)	50,54,54	1.66	9 (18%)

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	GTP	D	301	-	-	7/22/38/38	0/3/3/3
3	GTP	C	301	-	-	5/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	GTP	C2-N3	2.21	1.38	1.33
3	D	301	GTP	C2-N3	2.18	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	GTP	C5-C4-N3	-5.56	119.54	128.39
3	D	301	GTP	C5-C4-N3	-5.40	119.80	128.39
3	C	301	GTP	C2-N3-C4	4.90	120.74	112.30
3	D	301	GTP	C2-N3-C4	4.86	120.67	112.30
3	C	301	GTP	N9-C4-N3	3.77	133.48	125.95
3	D	301	GTP	N9-C4-N3	3.57	133.10	125.95
3	C	301	GTP	C2-N1-C6	-3.00	119.67	125.11
3	D	301	GTP	C2-N1-C6	-2.96	119.75	125.11
3	D	301	GTP	N9-C8-N7	-2.55	108.67	113.40
3	C	301	GTP	C5-C6-N1	2.54	119.72	113.25
3	D	301	GTP	C5-C6-N1	2.54	119.72	113.25
3	D	301	GTP	C8-N7-C5	2.53	108.77	104.26
3	C	301	GTP	C8-N7-C5	2.47	108.66	104.26
3	C	301	GTP	O6-C6-C5	-2.46	120.04	126.53
3	C	301	GTP	N9-C8-N7	-2.41	108.92	113.40
3	D	301	GTP	O6-C6-C5	-2.39	120.22	126.53
3	C	301	GTP	C3'-C2'-C1'	2.36	105.93	101.46
3	D	301	GTP	C3'-C2'-C1'	2.22	105.66	101.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	GTP	C5'-O5'-PA-O1A
3	D	301	GTP	C5'-O5'-PA-O3A
3	D	301	GTP	C5'-O5'-PA-O1A

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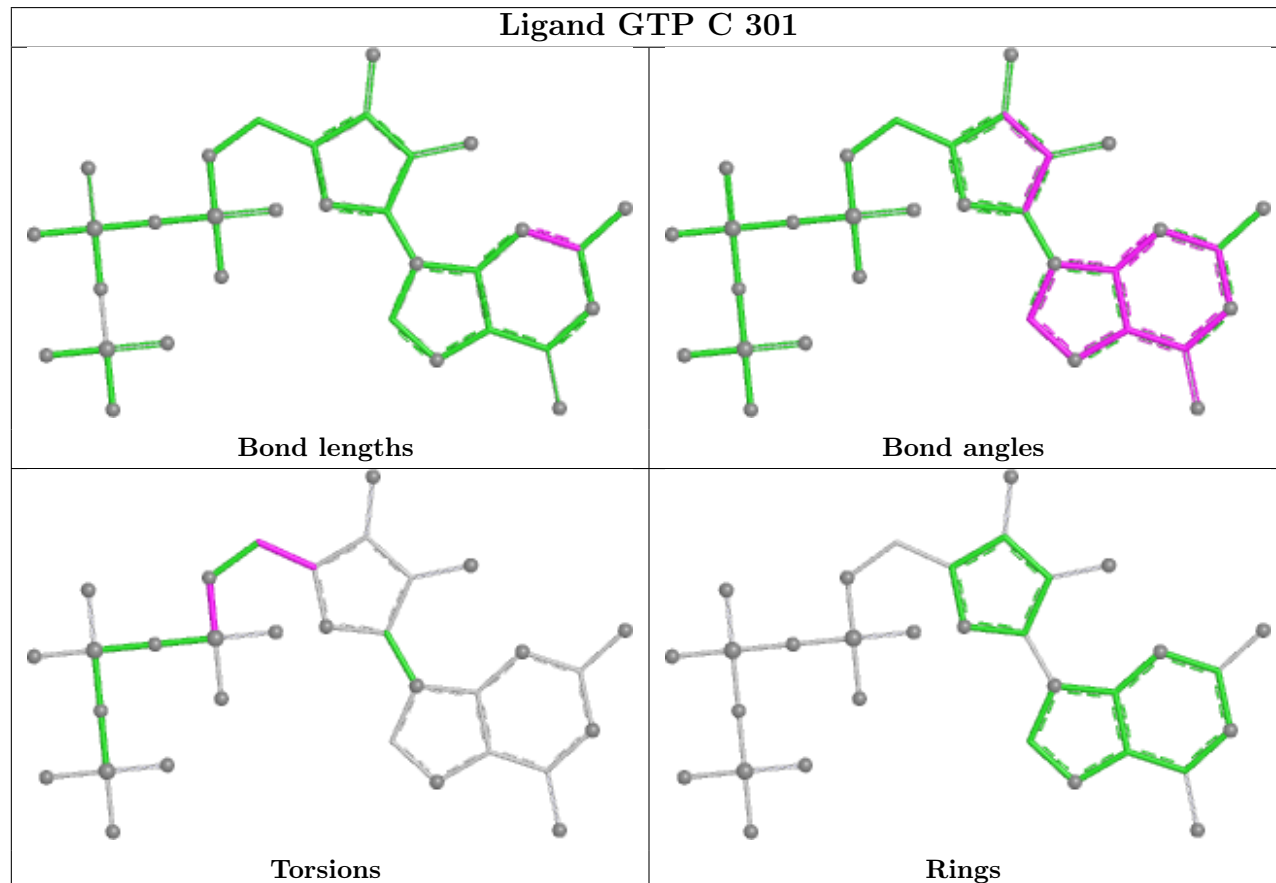
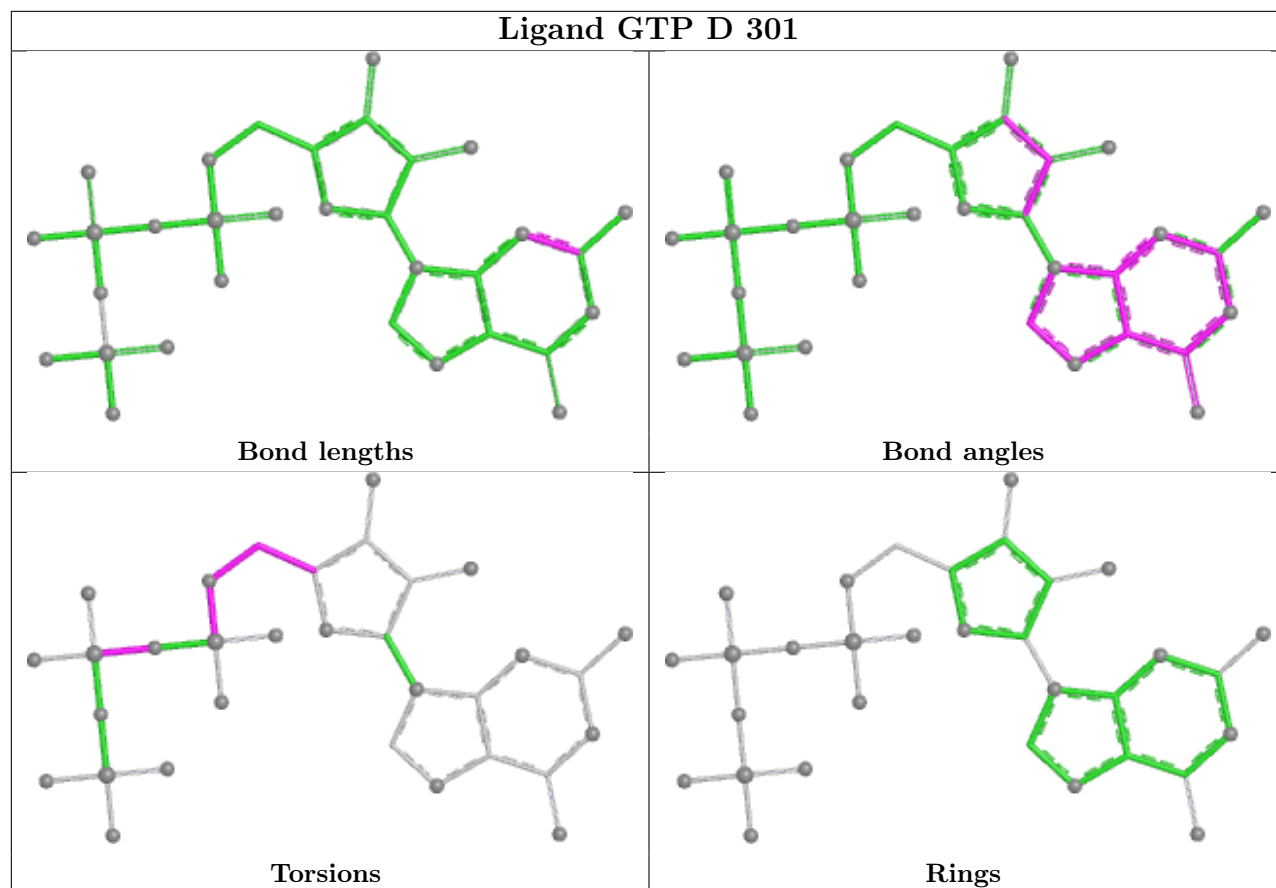
Mol	Chain	Res	Type	Atoms
3	C	301	GTP	O4'-C4'-C5'-O5'
3	D	301	GTP	C3'-C4'-C5'-O5'
3	C	301	GTP	C3'-C4'-C5'-O5'
3	D	301	GTP	O4'-C4'-C5'-O5'
3	C	301	GTP	C5'-O5'-PA-O3A
3	C	301	GTP	C5'-O5'-PA-O2A
3	D	301	GTP	C5'-O5'-PA-O2A
3	D	301	GTP	C4'-C5'-O5'-PA
3	D	301	GTP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	GTP	1	0
3	C	301	GTP	2	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](#)

There are no chain breaks in this entry.

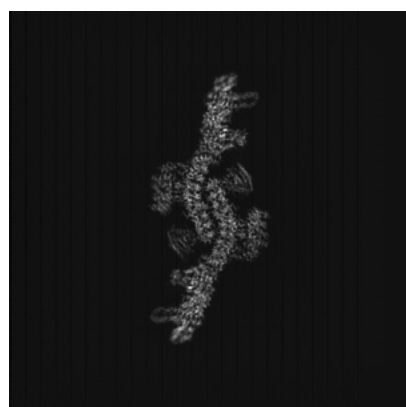
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28743. These allow visual inspection of the internal detail of the map and identification of artifacts.

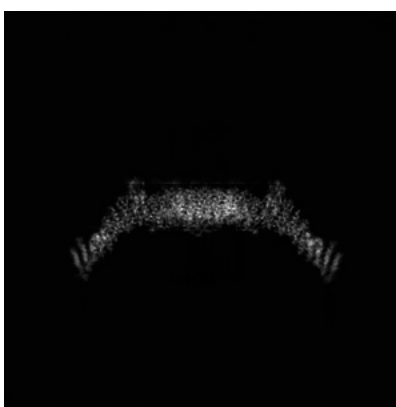
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

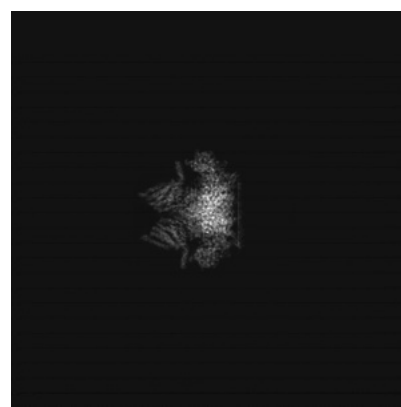
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

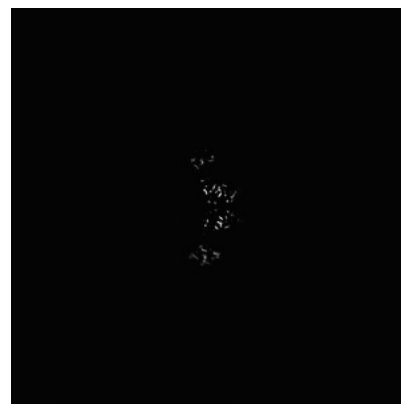
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

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: 256



Y Index: 274

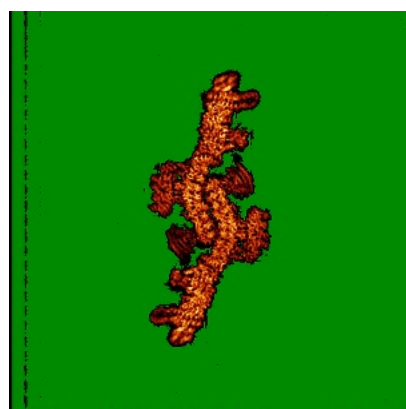


Z Index: 237

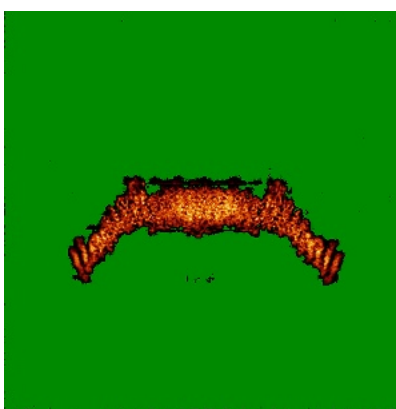
The images above show the largest variance slices of the map in three orthogonal directions.

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

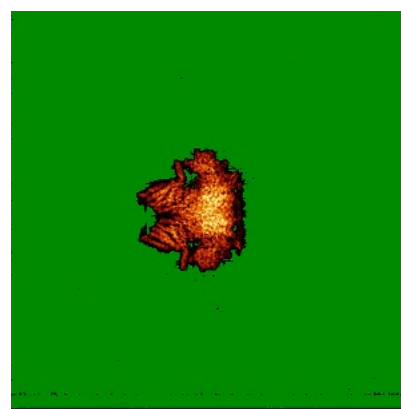
6.4.1 Primary map



X



Y

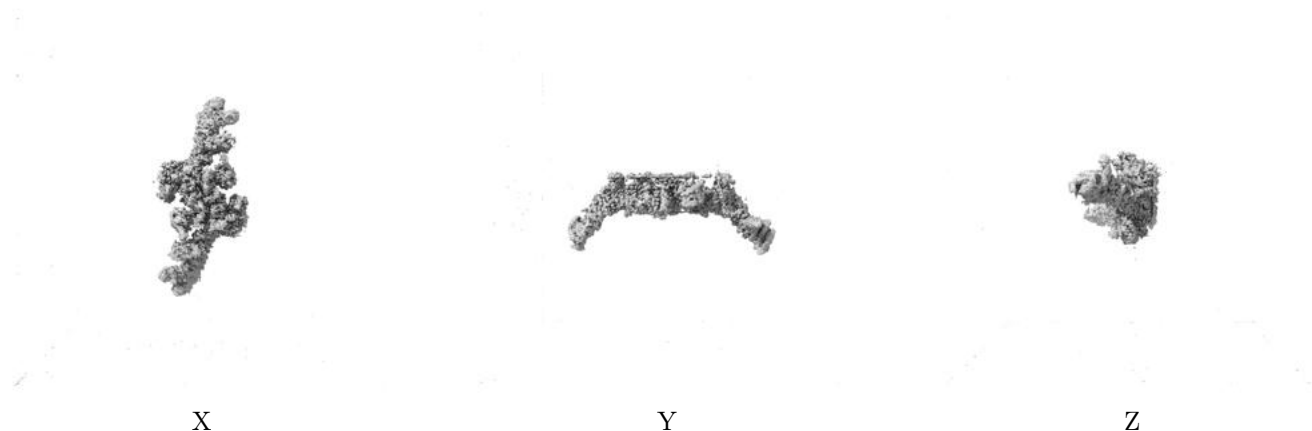


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

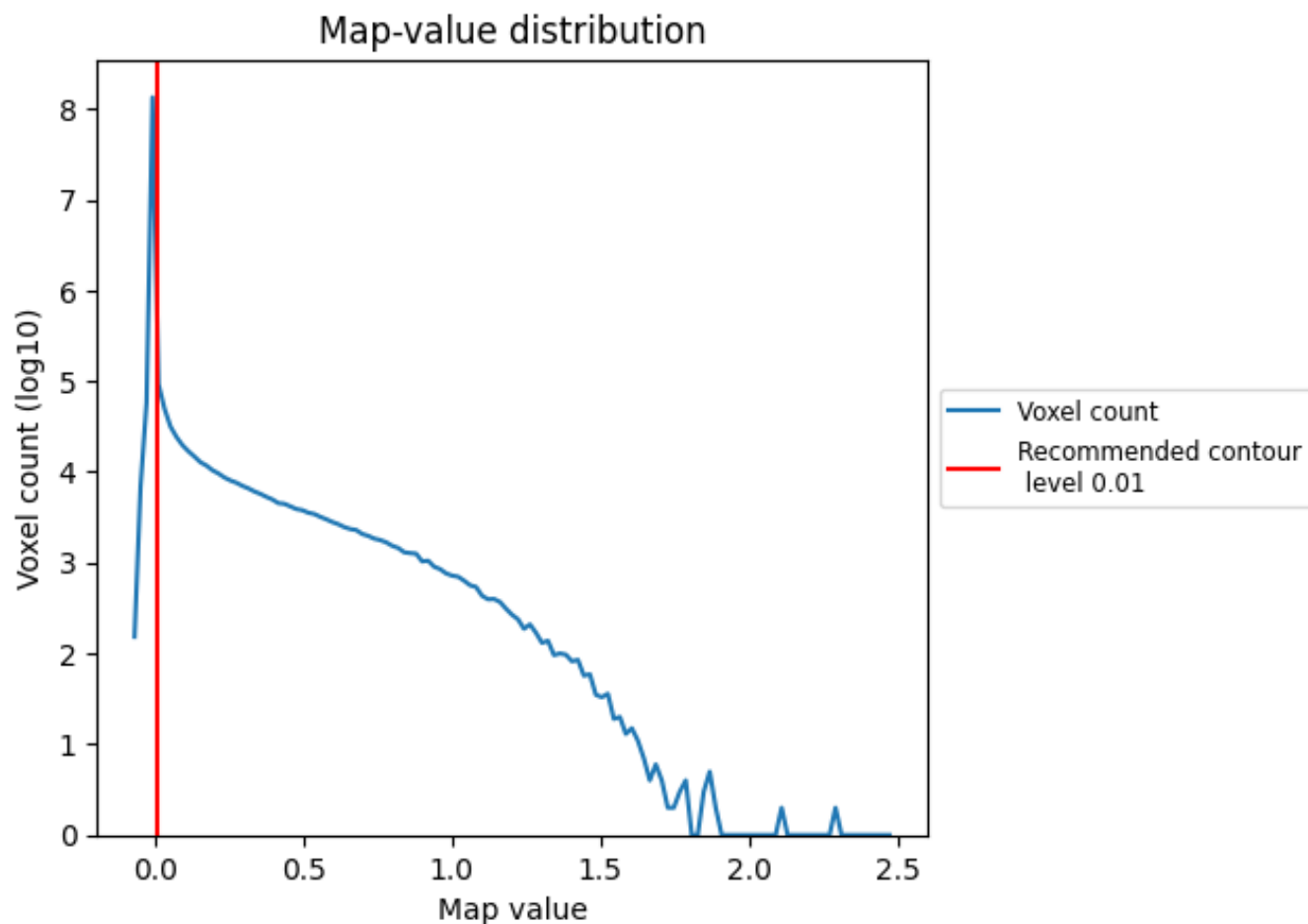
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

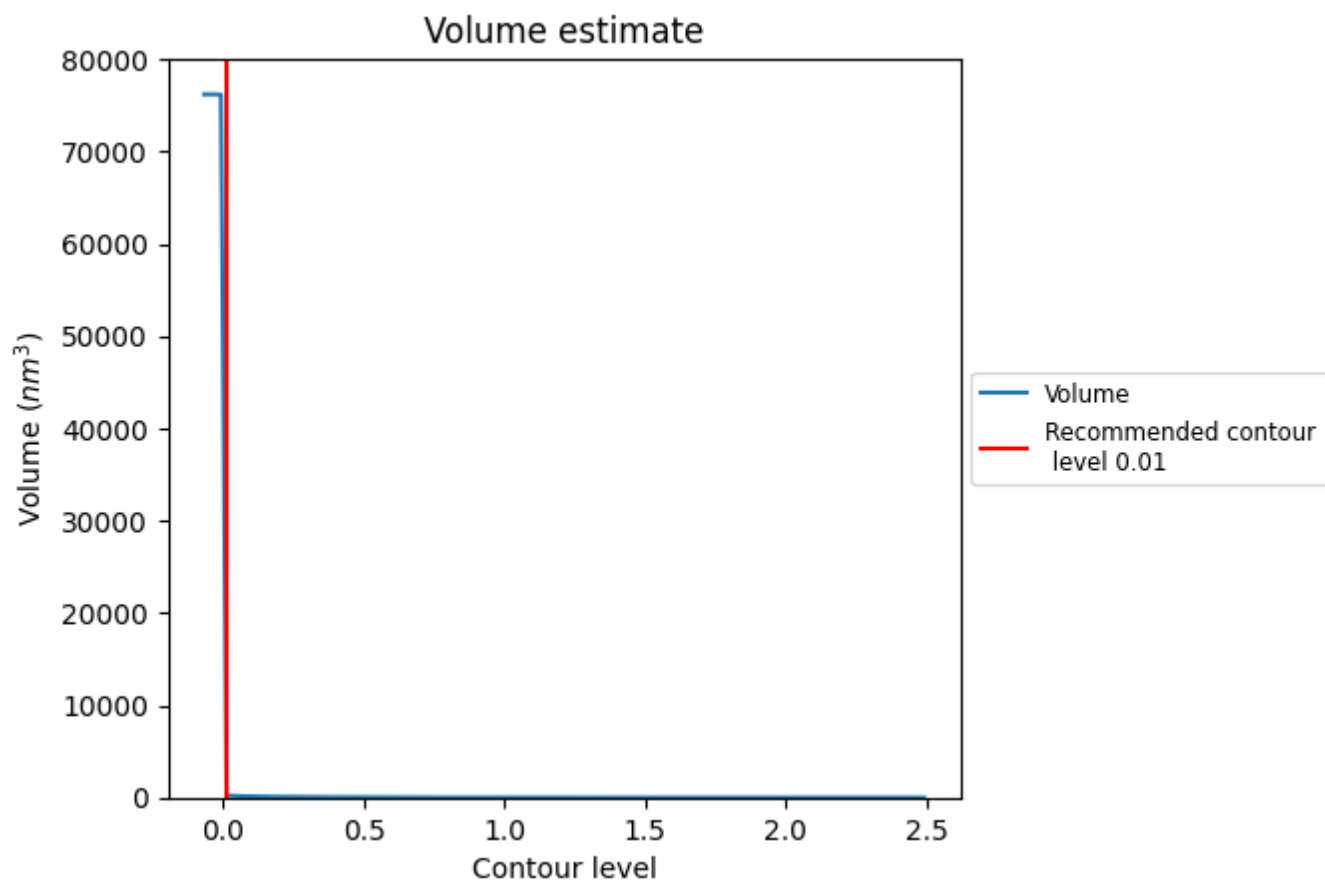
This section contains the results of statistical analysis of the map.

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.

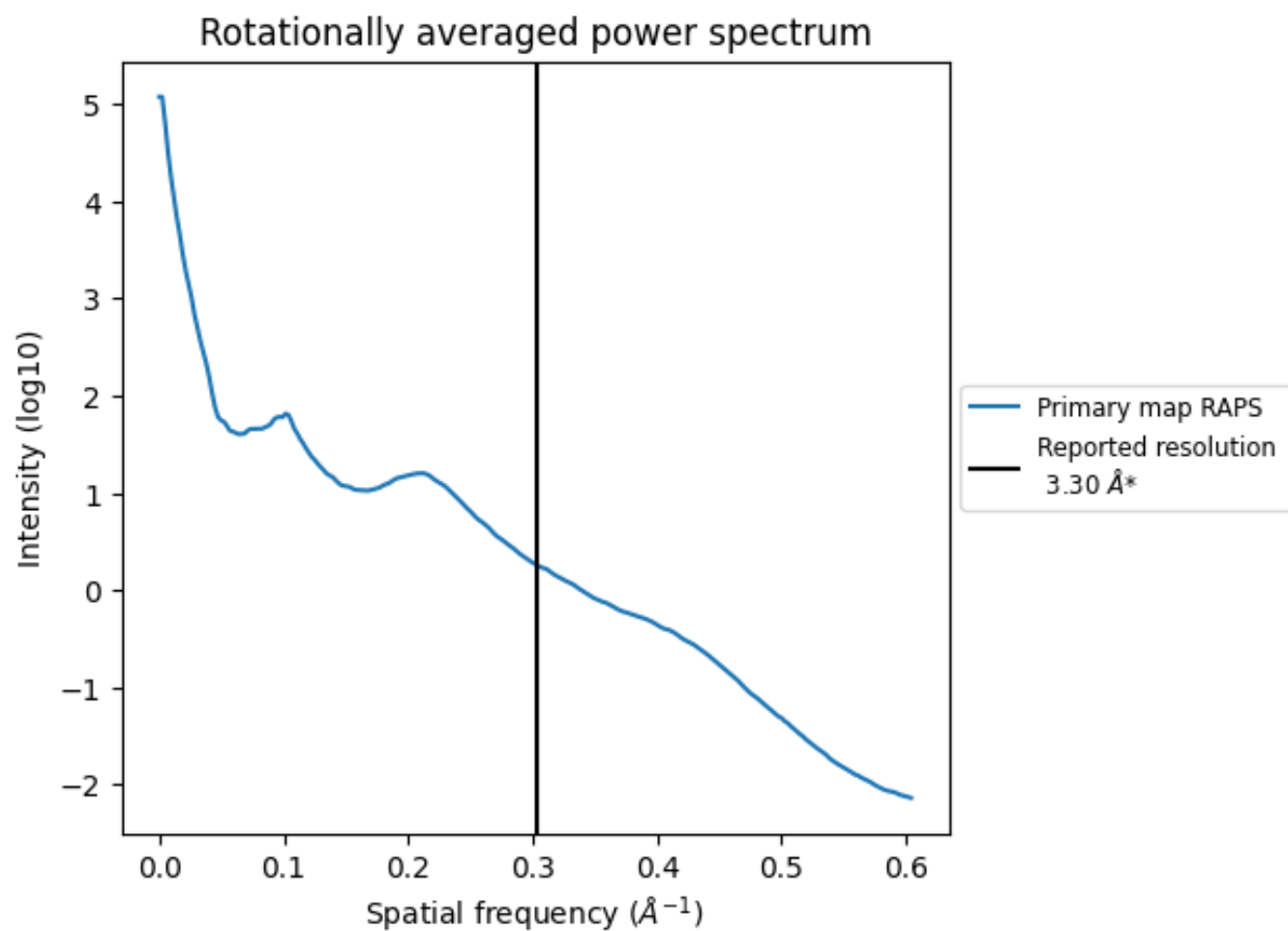
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 12200 nm^3 ; this corresponds to an approximate mass of 11021 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 0.303 Å⁻¹

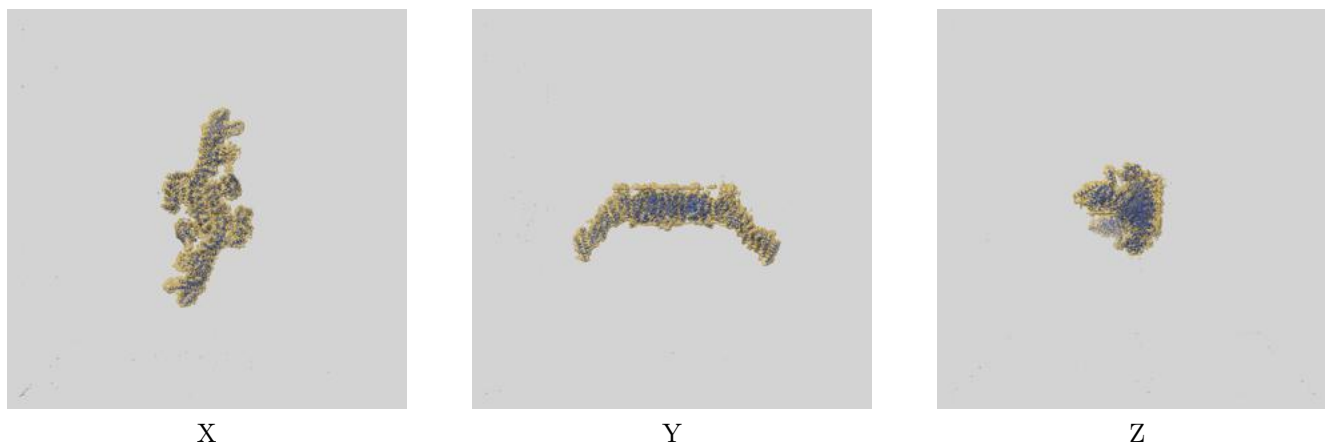
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

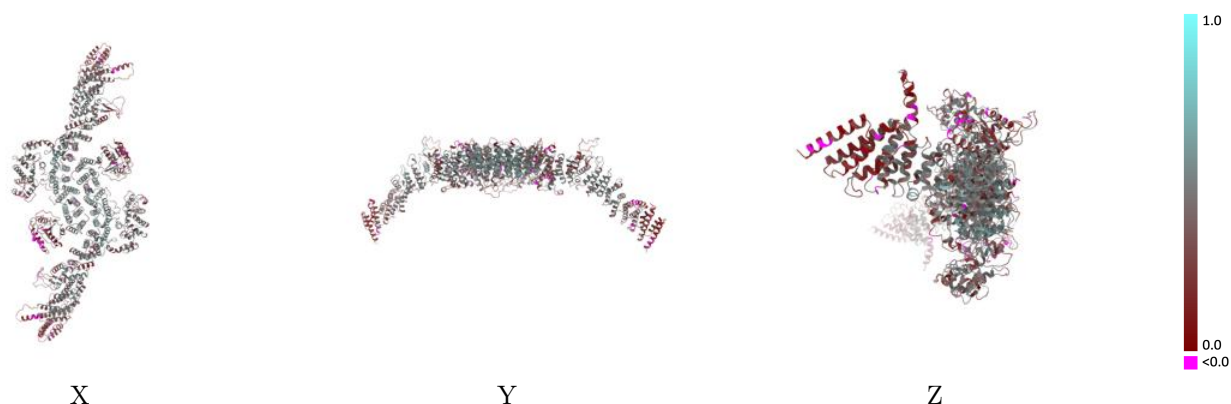
This section contains information regarding the fit between EMDB map EMD-28743 and PDB model 8EZJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



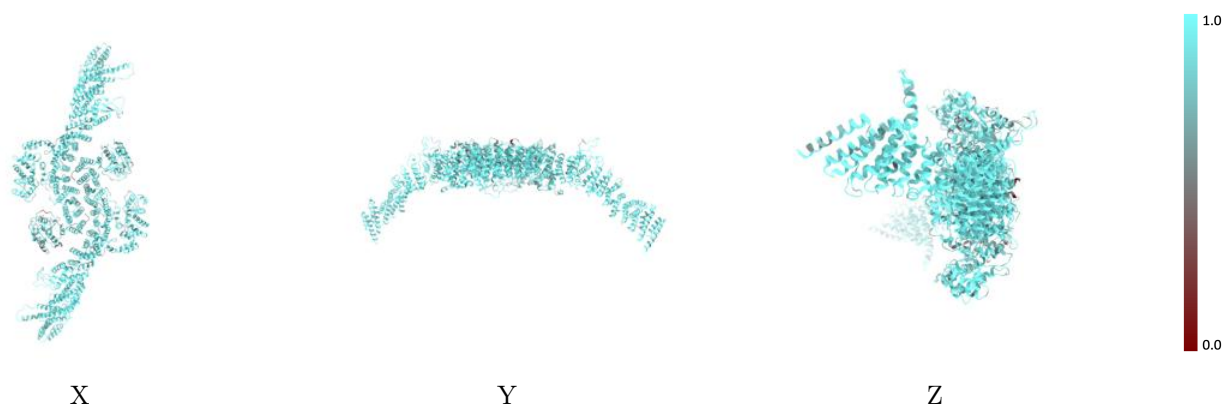
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



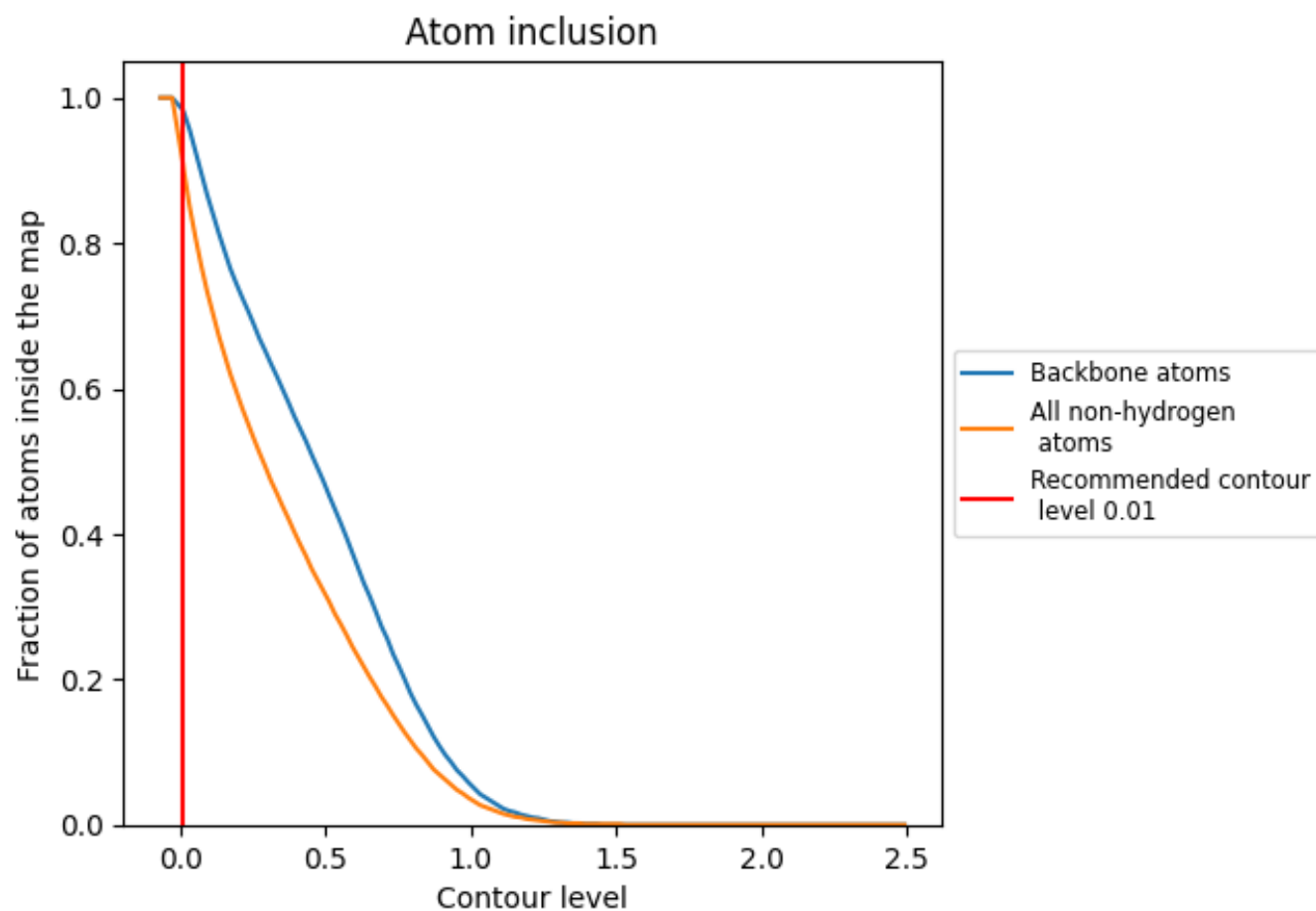
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.3990
A	0.9250	0.4160
B	0.9270	0.4140
C	0.7450	0.2500
D	0.8280	0.3040

