

Jun 11, 2024 – 06:38 PM JST

PDB ID	:	7VPZ
EMDB ID	:	EMD-32077
Title	:	Cryo-EM structure of Streptomyces coelicolor transcription initial complex
		with one Zur dimer
Authors	:	Yang, X.; Zheng, J.
Deposited on	:	2021-10-18
Resolution	:	4.14 Å(reported)
This is	s a I	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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.14 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)	${ m EM} { m structures} \ (\#{ m Entries})$
Clashscore	158937	4297
Ramachandran outliors	15/1571	4023
Sidachain antlian	154915	4023
Sidechain outliers	104010	3820
RNA backbone	4643	859

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 $\geq=3, 2, 1$ 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	Q	uality of cha	in	
1	А	340	55%	119	6 •	34%
1	В	340	• 61%		7% •	31%
2	С	1161	789	%		18% •
3	D	1307	81	1%		16% ·
4	Е	90	72%		13%	14%
5	F	531	47%	10%	43%	
6	М	159	18%		12%	18%



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Continued	trom	previous	paae
Contraca	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	p1000000	pagom

Mol	Chain	Length	Quality of chain	
6	Ν	159	7% 13%	18%
7	Ο	84	94%	6%
8	Р	84	83%	17%
9	Q	5	80%	20%



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 30593 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
1	А	226	Total 1742	C 1102	N 302	0 334	${S \atop 4}$	0	0
1	В	233	Total 1792	C 1131	N 309	О 347	${ m S}{ m 5}$	0	0

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

Mol	Chain	Residues		Α	toms			AltConf	Trace
2	С	1116	Total 8692	C 5450	N 1513	O 1698	S 31	0	0

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

Mol	Chain	Residues		Α	toms			AltConf	Trace
3	D	1259	Total	C	N 1707	0	S	0	0
			9840	0101	1787	1857	41		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1300	HIS	-	expression tag	UNP Q8CJT1
D	1301	HIS	-	expression tag	UNP Q8CJT1
D	1302	HIS	-	expression tag	UNP Q8CJT1
D	1303	HIS	-	expression tag	UNP Q8CJT1
D	1304	HIS	-	expression tag	UNP Q8CJT1
D	1305	HIS	-	expression tag	UNP Q8CJT1
D	1306	HIS	-	expression tag	UNP Q8CJT1
D	1307	HIS	-	expression tag	UNP Q8CJT1

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	Е	77	Total 597	C 382	N 98	0 117	0	0

• Molecule 5 is a protein called RNA polymerase principal sigma factor HrdB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	301	Total 2396	C 1509	N 426	0 454	${ m S} 7$	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P18183
F	-18	GLY	-	expression tag	UNP P18183
F	-17	SER	-	expression tag	UNP P18183
F	-16	SER	-	expression tag	UNP P18183
F	-15	HIS	-	expression tag	UNP P18183
F	-14	HIS	-	expression tag	UNP P18183
F	-13	HIS	-	expression tag	UNP P18183
F	-12	HIS	-	expression tag	UNP P18183
F	-11	HIS	-	expression tag	UNP P18183
F	-10	HIS	-	expression tag	UNP P18183
F	-9	SER	-	expression tag	UNP P18183
F	-8	SER	-	expression tag	UNP P18183
F	-7	GLY	-	expression tag	UNP P18183
F	-6	LEU	-	expression tag	UNP P18183
F	-5	VAL	-	expression tag	UNP P18183
F	-4	PRO	-	expression tag	UNP P18183
F	-3	ARG	-	expression tag	UNP P18183
F	-2 GLY - expression tag		UNP P18183		
F	-1	SER	-	expression tag	UNP P18183
F	0	HIS	-	expression tag	UNP P18183

• Molecule 6 is a protein called Putative metal uptake regulation protein.

Mol	Chain	Residues		At	oms			AltConf	Trace
6	М	131	Total 984	C 603	N 185	0 190	S 6	0	0
6	N	131	Total 984	C 603	N 185	O 190	S 6	0	0

There are 40 discrepancies between the modelled and reference sequences:



Chain	Residue Modelled Actual Comm			Comment	Reference
М	-19	MET	-	initiating methionine	UNP Q9L2H5
М	-18	GLY	-	expression tag	UNP Q9L2H5
М	-17	SER	-	expression tag	UNP Q9L2H5
М	-16	SER	-	expression tag	UNP Q9L2H5
М	-15	HIS	-	expression tag	UNP Q9L2H5
М	-14	HIS	-	expression tag	UNP Q9L2H5
М	-13	HIS	-	expression tag	UNP Q9L2H5
М	-12	HIS	-	expression tag	UNP Q9L2H5
М	-11	HIS	-	expression tag	UNP Q9L2H5
М	-10	HIS	-	expression tag	UNP Q9L2H5
М	-9	SER	-	expression tag	UNP Q9L2H5
М	-8	SER	-	expression tag	UNP Q9L2H5
М	-7	GLY	-	expression tag	UNP Q9L2H5
М	-6	LEU	-	expression tag	UNP Q9L2H5
М	-5	VAL	-	expression tag	UNP Q9L2H5
М	-4	PRO	-	expression tag	UNP Q9L2H5
М	-3	ARG	-	expression tag	UNP Q9L2H5
М	-2	GLY	-	expression tag	UNP Q9L2H5
М	-1	SER	-	expression tag	UNP Q9L2H5
М	0	HIS	-	expression tag	UNP Q9L2H5
N	-19	MET	-	initiating methionine	UNP Q9L2H5
N	-18	GLY	-	expression tag	UNP Q9L2H5
N	-17	SER	-	expression tag	UNP Q9L2H5
N	-16	SER	-	expression tag	UNP Q9L2H5
N	-15	HIS	-	expression tag	UNP Q9L2H5
N	-14	HIS	-	expression tag	UNP Q9L2H5
N	-13	HIS	-	expression tag	UNP Q9L2H5
N	-12	HIS	-	expression tag	UNP Q9L2H5
N	-11	HIS	-	expression tag	UNP Q9L2H5
N	-10	HIS	-	expression tag	UNP Q9L2H5
N	-9	SER	-	expression tag	UNP Q9L2H5
N	-8	SER	-	expression tag	UNP Q9L2H5
N	-7	GLY	-	expression tag	UNP Q9L2H5
N	-6	LEU	-	expression tag	UNP Q9L2H5
N	-5	VAL	-	expression tag	UNP Q9L2H5
N	-4	PRO	-	expression tag	UNP Q9L2H5
N	-3	ARG	-	expression tag	UNP Q9L2H5
N	-2	GLY	-	expression tag	UNP Q9L2H5
N	-1	SER	-	expression tag	UNP Q9L2H5
N	0	HIS	-	expression tag	UNP Q9L2H5

• Molecule 7 is a DNA chain called DNA (84-MER).



Mol	Chain	Residues		A	toms			AltConf	Trace
7	0	84	Total 1714	C 810	N 315	O 505	Р 84	0	0

• Molecule 8 is a DNA chain called DNA (84-MER).

Mol	Chain	Residues		AltConf	Trace				
8	Р	84	Total 1729	C 815	N 325	O 505	Р 84	0	0

• Molecule 9 is a RNA chain called RNA.

Mol	Chain	Residues		\mathbf{At}	\mathbf{oms}			AltConf	Trace
9	Q	5	Total 108	C 49	N 22	O 33	Р 4	0	0

• Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
10	D	1	Total Mg 1 1	0

• Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
11	D	2	Total Zn 2 2	0
11	М	3	Total Zn 3 3	0
11	Ν	3	Total Zn 3 3	0



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: DNA-directed RNA polymerase subunit alpha



Y330	000A	CCCV	T339	E340 T244	1341	E348	1301	V351 E352	-	H358		1364	R387		1404	DA DO		F417		S423	M426		N430		R439	L444		R453	V461		Y466	R468		1472	L482	-	1492	N493	F497	1498		V505	G5 08	H H	1510 A519	-
D523	A E 2 O	000H	R549	R550	D555		D560	V562	-	D566		S5/4 VE76	A576	T577	A578	M579	L604		E608	8609	T614		E617		V627	E631	K632	A633	V636		V639	3040 A641		1644	N648	D649	D650	G651	L658	A659	K660	NG7 1	q672	02011	0/0/	E684
-	V687	L000 A689	D690	an an an	060N	L701			N7 16		L723	S/ 24	D731		V743	D767		E765	V7 66	L767	A/ 00	D771	-	1775	I776	L788		L800	E804		R808	G812		5822 1 623	K824	-	R841	Dovo	1040	R856		K864	A872		V000 I881	<mark>S882</mark>
-	E888	06890 W890		L903	N304	M912	N913 B014		V917		1920		H-70H	V932	-	L935	E938	-	R942	L943	G947	A948	D949	K950	V951 E952	4001	A958	T959	A965		E969	L974		T977	N980	R981	_	P989	K992	-	I1008	1 1018		R1029	T1031	-
M1036	11037		<mark>q1047</mark>	F1048	A1060	-	Y1064	E1072	-	K1077	S1078		E1095	N1096	11097	E1104	S1105	F1106	K1107	V1108	F110A	L1116	-	E1131	MET ARG	ASP	THR	ASP	ASP	VAL	PHE	ALA	ALA	GLU	TEU	GLY	ILE	ASP	SER	ARG	ARG	GLU	SER	SER	GLU	GLU
VAL																																														

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



• Molecule 4: DNA-directed RNA polymerase subunit omega







Chain O:	94%	6%
C1 A2 G1 1 G1 1 G7 1 G7 1 G7 2 C8 4 C8 4		
• Molecule 8: DNA (84	4-MER)	
Chain P:	83%	17%
G1 C13 C13 C13 C13 C13 C13 C13 C13 C13 C13	T61 662 663 763 783 783 783 684 783 684 783 684 684 684 684 684 684 685 684 685 686 686 686 686 686 686 686 686 686	
• Molecule 9: RNA		
Chain Q:	80%	20%
8		



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21494	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40, 40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k), GATAN	Depositor
	K3 BIOQUANTUM (6k x 4k)	
Maximum map value	2.751	Depositor
Minimum map value	-1.584	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.29	0/1768	0.58	0/2400
1	В	0.28	0/1818	0.59	0/2467
2	С	0.29	0/8848	0.56	0/11982
3	D	0.28	0/9998	0.59	0/13490
4	Е	0.30	0/607	0.53	0/826
5	F	0.27	0/2431	0.56	0/3277
6	М	0.26	0/1001	0.59	0/1355
6	Ν	0.24	0/1001	0.51	0/1355
7	0	0.68	0/1920	0.95	0/2959
8	Р	0.67	0/1940	0.90	0/2994
9	Q	0.24	0/121	0.55	0/188
All	All	0.35	0/31453	0.63	0/43293

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	А	1742	0	1796	21	0
1	В	1792	0	1841	22	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	8692	0	8632	133	0
3	D	9846	0	10017	145	0
4	Е	597	0	604	10	0
5	F	2396	0	2453	33	0
6	М	984	0	947	14	0
6	Ν	984	0	947	13	0
7	0	1714	0	940	7	0
8	Р	1729	0	940	17	0
9	Q	108	0	55	0	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
11	М	3	0	0	0	0
11	N	3	0	0	0	0
All	All	30593	0	29172	373	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 6.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:140:VAL:HG21	2:C:404:ILE:HD11	1.57	0.87
2:C:912:MET:SD	3:D:811:GLN:NE2	2.50	0.84
2:C:364:ILE:HD11	2:C:492:ILE:HD12	1.64	0.78
1:B:55:ARG:NH1	1:B:56:ILE:O	2.18	0.77
3:D:502:PRO:HG3	8:P:15:DG:H22	1.51	0.74
3:D:665:ARG:NE	3:D:680:ASP:O	2.21	0.74
3:D:579:GLN:OE1	3:D:803:ARG:NH1	2.21	0.73
2:C:549:ARG:NH2	2:C:555:ASP:OD2	2.21	0.73
2:C:841:ARG:NH2	2:C:848:PRO:O	2.22	0.72
3:D:751:VAL:HG11	3:D:768:GLU:OE2	1.88	0.72
4:E:10:GLY:N	4:E:13:ASN:OD1	2.21	0.72
2:C:200:LEU:HD13	2:C:214:ILE:HD13	1.71	0.72
6:M:27:GLU:O	6:M:77:ARG:NE	2.22	0.72
2:C:1072:GLU:OE2	3:D:547:LEU:N	2.23	0.72
3:D:76:GLU:OE2	3:D:76:GLU:N	2.23	0.72
6:N:78:ARG:NH1	6:N:79:CYS:O	2.23	0.72
6:N:15:GLN:NE2	7:0:11:DG:OP2	2.24	0.70
2:C:765:GLU:N	2:C:765:GLU:OE1	2.24	0.70
2:C:771:ASP:N	2:C:775:ILE:O	2.23	0.70
3:D:1048:VAL:O	3:D:1085:GLY:N	2.25	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:C:1029:ARG:NH1	2:C:1048:PHE:O	2.25	0.70
6:N:77:ARG:NH1	6:N:79:CYS:SG	2.65	0.69
2:C:339:THR:OG1	2:C:340:GLU:OE1	2.11	0.69
2:C:800:LEU:HD12	2:C:804:GLU:OE1	1.92	0.69
3:D:357:LEU:HD21	5:F:309:LEU:HD21	1.74	0.69
4:E:65:GLU:OE1	4:E:65:GLU:N	2.26	0.68
2:C:617:GLU:OE1	2:C:617:GLU:N	2.27	0.67
3:D:143:ARG:NH1	3:D:250:THR:O	2.28	0.67
2:C:924:TRP:HZ3	2:C:977:THR:HG21	1.60	0.67
5:F:301:LEU:HA	5:F:304:ILE:HD12	1.77	0.67
2:C:256:GLN:N	2:C:256:GLN:OE1	2.29	0.66
3:D:920:LEU:HG	3:D:938:LEU:HD21	1.77	0.66
3:D:923:ASP:OD1	3:D:934:ALA:N	2.28	0.66
3:D:973:TYR:O	3:D:1135:LYS:NZ	2.20	0.66
2:C:33:GLU:OE1	2:C:33:GLU:N	2.29	0.66
2:C:161:ARG:NH2	2:C:423:SER:O	2.29	0.66
2:C:364:ILE:CD1	2:C:492:ILE:HD12	2.27	0.65
3:D:963:GLU:OE2	3:D:965:GLN:NE2	2.30	0.64
2:C:1079:ASP:OD2	3:D:420:LYS:NZ	2.28	0.64
3:D:345:ARG:NH2	5:F:348:THR:O	2.31	0.64
2:C:822:SER:O	2:C:824:LYS:NZ	2.31	0.64
3:D:173:ARG:NE	3:D:208:LEU:HD23	2.12	0.64
2:C:731:ASP:OD1	2:C:864:LYS:NZ	2.27	0.64
3:D:96:GLU:O	3:D:351:ASN:ND2	2.31	0.63
2:C:724:SER:OG	2:C:890:MET:SD	2.53	0.63
6:N:28:GLU:OE1	6:N:30:ARG:NH2	2.32	0.62
1:B:224:GLU:N	1:B:224:GLU:OE1	2.32	0.62
2:C:358:HIS:NE2	2:C:519:ALA:O	2.31	0.62
3:D:502:PRO:HB3	8:P:15:DG:N2	2.14	0.61
2:C:453:ARG:HA	7:O:71:DG:H1'	1.81	0.61
2:C:523:ASP:OD2	2:C:550:ARG:NE	2.33	0.61
2:C:508:GLY:N	2:C:560:ASP:OD1	2.34	0.60
5:F:472:LEU:HD12	8:P:48:DG:OP2	2.00	0.60
1:A:152:ASN:ND2	1:A:152:ASN:O	2.33	0.60
3:D:587:PHE:O	3:D:622:GLN:NE2	2.33	0.60
4:E:36:ARG:NE	4:E:74:GLU:OE1	2.35	0.60
3:D:671:LEU:HD21	3:D:714:ALA:CB	2.31	0.60
1:B:108:ALA:N	1:B:121:PRO:O	2.35	0.60
2:C:196:ARG:HB3	2:C:295:ASP:HB3	1.82	0.60
3:D:1044:ALA:HA	3:D:1090:VAL:HG12	1.84	0.60
2:C:980:ASN:OD1	2:C:981:ARG:N	2.34	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:608:GLU:OE2	2:C:609:SER:N	2.35	0.60
2:C:1077:LYS:NZ	3:D:545:LEU:O	2.25	0.60
2:C:1116:LEU:HD13	3:D:105:TRP:CH2	2.37	0.60
2:C:716:ASN:O	2:C:904:ASN:ND2	2.35	0.59
3:D:1189:GLN:NE2	3:D:1190:LEU:O	2.35	0.59
3:D:884:GLU:OE2	3:D:884:GLU:N	2.32	0.59
2:C:952:GLU:OE1	2:C:952:GLU:N	2.35	0.59
2:C:650:ASP:OD1	2:C:651:GLY:N	2.35	0.59
3:D:618:ASP:OD1	3:D:619:LEU:N	2.36	0.59
6:M:55:LEU:HD13	6:M:76:TYR:HE2	1.66	0.59
3:D:1029:LEU:HD12	3:D:1117:LEU:HD23	1.85	0.59
2:C:23:ILE:O	2:C:958:ALA:N	2.36	0.59
6:M:28:GLU:OE2	6:M:30:ARG:NH2	2.36	0.59
2:C:444:LEU:HD21	2:C:482:LEU:HD13	1.83	0.58
2:C:631:GLU:N	2:C:631:GLU:OE1	2.36	0.58
3:D:586:PHE:O	3:D:590:THR:OG1	2.21	0.58
3:D:671:LEU:HD21	3:D:714:ALA:HB3	1.84	0.58
3:D:493:GLU:OE2	4:E:10:GLY:N	2.37	0.58
3:D:527:LEU:HD21	3:D:712:LYS:HB2	1.84	0.58
1:B:154:GLN:N	1:B:154:GLN:OE1	2.37	0.58
7:O:72:DG:H1	8:P:13:DC:H42	1.52	0.57
2:C:173:VAL:HG12	2:C:192:ILE:HG22	1.87	0.57
2:C:341:THR:N	2:C:348:GLU:OE2	2.36	0.57
2:C:882:SER:OG	3:D:432:VAL:O	2.22	0.57
3:D:626:ASP:OD1	3:D:627:ILE:N	2.38	0.57
6:N:27:GLU:OE1	6:N:77:ARG:NH2	2.37	0.57
3:D:525:HIS:CE1	3:D:527:LEU:HD23	2.40	0.57
3:D:238:GLU:OE1	3:D:238:GLU:N	2.37	0.56
2:C:1036:MET:HB3	5:F:424:ASP:HB3	1.87	0.56
3:D:502:PRO:CG	8:P:15:DG:H22	2.18	0.56
5:F:359:ILE:HD13	5:F:396:VAL:HG12	1.87	0.56
3:D:487:LEU:HD22	3:D:516:LEU:HD11	1.88	0.56
2:C:949:ASP:OD1	2:C:950:LYS:N	2.39	0.55
3:D:1058:LYS:NZ	3:D:1059:ILE:O	2.40	0.55
2:C:352:GLU:N	2:C:352:GLU:OE1	2.40	0.55
2:C:671:ASN:OD1	2:C:672:GLN:N	2.39	0.55
2:C:942:ARG:NH2	2:C:969:GLU:OE2	2.40	0.55
6:M:123:THR:OG1	6:N:125:GLU:O	2.25	0.55
3:D:502:PRO:CB	8:P:15:DG:N2	2.69	0.55
5:F:229:ASN:O	5:F:232:GLN:N	2.40	0.55
8:P:21:DG:H2'	8:P:22:DG:C8	2.41	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:C:430:ASN:HD22	2:C:701:LEU:HD22	1.72	0.54
2:C:472:ILE:CD1	2:C:577:THR:HG21	2.37	0.54
1:A:79:ASN:O	1:A:82:GLN:NE2	2.40	0.54
3:D:770:ILE:HD12	3:D:826:THR:HG21	1.88	0.54
3:D:1261:ALA:HB2	4:E:79:LEU:HD21	1.88	0.54
5:F:354:HIS:O	5:F:358:VAL:HG23	2.07	0.54
1:A:184:GLU:OE2	1:A:184:GLU:N	2.35	0.54
1:A:200:GLN:OE1	1:A:200:GLN:N	2.41	0.54
3:D:277:LEU:HD21	3:D:295:ARG:HE	1.72	0.54
2:C:212:VAL:O	2:C:213:ARG:NE	2.40	0.54
1:A:154:GLN:OE1	1:A:154:GLN:N	2.40	0.54
3:D:1060:VAL:HG13	3:D:1069:GLU:OE2	2.08	0.54
3:D:938:LEU:HD22	3:D:942:LEU:HD22	1.91	0.53
6:M:66:VAL:HG12	6:M:76:TYR:CE1	2.43	0.53
2:C:888:GLU:OE2	2:C:888:GLU:N	2.40	0.53
1:A:170:PRO:O	1:A:198:THR:OG1	2.21	0.53
6:N:81:THR:OG1	6:N:98:GLU:OE1	2.27	0.53
2:C:138:GLN:NE2	2:C:139:THR:O	2.41	0.53
5:F:413:ASP:O	5:F:416:SER:OG	2.20	0.53
3:D:349:ASN:ND2	5:F:345:GLN:OE1	2.41	0.52
3:D:763:GLU:O	3:D:766:THR:OG1	2.22	0.52
3:D:1256:GLU:OE1	3:D:1256:GLU:N	2.43	0.52
4:E:32:TYR:CE2	4:E:75:ILE:HD12	2.44	0.52
6:N:83:ASP:O	6:N:85:HIS:ND1	2.42	0.52
2:C:209:MET:SD	2:C:252:LYS:NZ	2.77	0.52
5:F:215:VAL:HG22	5:F:301:LEU:HB2	1.92	0.52
2:C:472:ILE:HD13	2:C:577:THR:HG21	1.92	0.52
2:C:203:GLU:N	2:C:203:GLU:OE1	2.43	0.51
3:D:128:VAL:HG21	3:D:135:MET:SD	2.50	0.51
2:C:85:GLU:O	2:C:387:ARG:NH1	2.43	0.51
2:C:461:VAL:HG23	3:D:852:ARG:HD2	1.92	0.51
6:M:83:ASP:O	6:M:85:HIS:ND1	2.37	0.51
2:C:992:LYS:HZ3	3:D:725:THR:CB	2.23	0.51
1:A:69:VAL:HG13	1:A:128:LEU:HD23	1.92	0.51
2:C:579:MET:O	2:C:614:THR:OG1	2.20	0.51
5:F:459:SER:O	5:F:463:GLY:N	2.43	0.51
2:C:237:LEU:O	2:C:241:GLY:N	2.43	0.51
3:D:809:MET:HA	3:D:812:ILE:HG22	1.91	0.51
2:C:175:PHE:CE1	2:C:190:ALA:HB2	2.46	0.51
5:F:485:ARG:HB2	7:O:34:DT:H71	1.92	0.51
3:D:879:VAL:O	3:D:879:VAL:HG13	2.11	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:C:872:ALA:HB3	2:C:1018:LEU:HD11	1.93	0.50
1:B:158:GLU:OE1	1:B:158:GLU:N	2.44	0.50
8:P:62:DG:H2"	8:P:63:DA:C8	2.46	0.50
3:D:888:THR:OG1	3:D:889:GLU:N	2.44	0.50
2:C:213:ARG:NH2	2:C:218:ARG:O	2.40	0.50
5:F:490:GLU:O	5:F:493:THR:OG1	2.28	0.50
2:C:156:ILE:HD13	2:C:417:PHE:HB3	1.94	0.50
4:E:9:GLU:N	4:E:9:GLU:OE1	2.45	0.50
2:C:676:VAL:HG21	2:C:688:LEU:CD1	2.42	0.50
3:D:210:ASP:O	3:D:213:GLN:NE2	2.44	0.49
1:A:186:ARG:HG3	1:B:150:VAL:HG21	1.93	0.49
3:D:644:ARG:HE	3:D:645:GLU:H	1.60	0.49
2:C:330:TYR:CZ	2:C:351:VAL:HG23	2.46	0.49
2:C:1064:TYR:OH	3:D:506:ARG:O	2.20	0.49
5:F:391:GLU:OE1	5:F:391:GLU:N	2.45	0.49
5:F:457:VAL:HB	5:F:486:ILE:HD11	1.94	0.49
1:B:60:LEU:HD22	1:B:159:ILE:HD13	1.93	0.49
2:C:408:PRO:HG3	8:P:26:DG:H8	1.76	0.49
1:B:39:ARG:O	1:B:43:LEU:HD23	2.12	0.49
2:C:530:ALA:HB2	2:C:566:ASP:HB2	1.94	0.49
3:D:588:LEU:HD21	3:D:664:GLY:O	2.12	0.49
3:D:976:SER:HB2	3:D:983:VAL:HG12	1.93	0.49
6:M:55:LEU:HD13	6:M:76:TYR:CE2	2.45	0.49
3:D:278:ARG:HH21	3:D:296:LEU:HD22	1.78	0.49
1:A:64:THR:OG1	1:A:65:THR:N	2.46	0.48
1:A:207:ALA:O	1:A:210:SER:OG	2.27	0.48
1:B:69:VAL:HG22	1:B:128:LEU:CD1	2.43	0.48
3:D:876:SER:O	3:D:879:VAL:HG12	2.12	0.48
6:N:55:LEU:HD21	6:N:76:TYR:CD1	2.47	0.48
6:N:68:ARG:NH2	6:N:72:GLY:O	2.46	0.48
3:D:89:ARG:N	3:D:323:ASP:OD2	2.46	0.48
2:C:808:ARG:O	2:C:812:GLY:N	2.47	0.48
2:C:1106:PHE:CZ	3:D:10:LEU:HD21	2.48	0.48
3:D:334:ARG:NH2	5:F:402:GLU:O	2.47	0.48
3:D:807:MET:SD	3:D:807:MET:N	2.86	0.48
1:B:39:ARG:NE	1:B:174:VAL:O	2.47	0.48
3:D:1203:TRP:NE1	3:D:1226:ASP:HB2	2.29	0.48
3:D:1233:GLU:OE1	3:D:1233:GLU:N	2.41	0.48
2:C:633:ALA:N	2:C:684:GLU:OE2	2.47	0.48
2:C:992:LYS:HZ1	2:C:1008:ILE:HA	1.78	0.48
3:D:1218:ASP:HA	3:D:1221:ILE:HG22	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:262:LEU:HD21	2:C:280:ALA:HB3	1.94	0.48
2:C:723:LEU:HD23	2:C:881:ILE:HD12	1.96	0.48
2:C:959:THR:HG23	2:C:959:THR:O	2.14	0.48
3:D:501:ALA:HB3	3:D:502:PRO:HD3	1.96	0.48
6:M:84:HIS:HE2	6:M:122:HIS:CE1	2.24	0.48
2:C:286:ASN:HA	2:C:290:ASN:HB2	1.96	0.48
2:C:493:ASN:N	2:C:497:PHE:O	2.40	0.48
2:C:914:PRO:O	2:C:917:VAL:HG12	2.14	0.48
3:D:1203:TRP:CD1	3:D:1226:ASP:HB2	2.49	0.48
5:F:279:LEU:HD23	5:F:311:LEU:HD22	1.96	0.48
2:C:160:GLU:O	2:C:426:MET:HB3	2.14	0.47
2:C:641:ALA:HB1	2:C:660:LYS:NZ	2.29	0.47
2:C:91:MET:SD	2:C:92:SER:N	2.87	0.47
2:C:505:VAL:HG11	2:C:562:VAL:HG23	1.96	0.47
3:D:596:SER:O	3:D:598:LYS:N	2.47	0.47
3:D:1089:GLU:N	3:D:1089:GLU:OE1	2.46	0.47
1:B:42:LEU:HD23	1:B:171:VAL:HG21	1.96	0.47
3:D:27:GLU:N	3:D:51:ILE:HD12	2.30	0.47
3:D:740:ILE:HD12	3:D:779:GLU:OE1	2.15	0.47
4:E:32:TYR:CZ	4:E:75:ILE:HD12	2.49	0.47
8:P:62:DG:H2"	8:P:63:DA:N7	2.30	0.47
2:C:707:VAL:HG21	2:C:903:LEU:HD12	1.97	0.47
3:D:506:ARG:N	3:D:995:GLN:OE1	2.48	0.47
3:D:1162:GLU:N	3:D:1162:GLU:OE1	2.48	0.47
3:D:1172:GLU:OE1	3:D:1175:ARG:NH1	2.47	0.47
7:0:71:DG:OP1	7:O:72:DG:P	2.72	0.47
2:C:330:TYR:CE1	2:C:351:VAL:HG23	2.50	0.47
2:C:767:LEU:HD12	2:C:767:LEU:O	2.14	0.47
3:D:304:GLN:NE2	3:D:305:THR:HG23	2.29	0.47
2:C:25:PHE:HD2	2:C:965:ALA:HB2	1.79	0.47
8:P:60:DC:H2'	8:P:61:DT:H72	1.97	0.47
2:C:200:LEU:HD12	2:C:213:ARG:O	2.15	0.46
2:C:468:ARG:HG2	2:C:498:ILE:HB	1.97	0.46
1:B:69:VAL:HG22	1:B:128:LEU:HD13	1.97	0.46
1:B:39:ARG:HE	1:B:43:LEU:HD21	1.79	0.46
3:D:830:PRO:O	3:D:832:LYS:NZ	2.40	0.46
1:B:137:GLU:OE1	1:B:137:GLU:N	2.49	0.46
2:C:209:MET:SD	2:C:249:THR:HG22	2.56	0.46
1:A:214:THR:O	1:A:218:LEU:HD23	2.16	0.46
2:C:1047:GLN:N	2:C:1047:GLN:OE1	2.49	0.46
3:D:142:GLU:OE1	3:D:142:GLU:N	2.43	0.46



	the page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:674:GLU:N	3:D:674:GLU:OE1	2.44	0.46
2:C:86:ASP:OD2	2:C:88:SER:OG	2.34	0.46
2:C:636:VAL:HG11	2:C:639:VAL:HG13	1.98	0.46
1:A:148:SER:OG	1:A:151:GLN:OE1	2.34	0.46
2:C:265:ILE:O	2:C:269:LEU:HD23	2.16	0.46
2:C:140:VAL:CG2	2:C:404:ILE:HD11	2.35	0.46
2:C:917:VAL:HA	2:C:920:ILE:HG22	1.97	0.46
2:C:1108:VAL:HG13	3:D:324:LEU:HD22	1.97	0.46
5:F:466:ASP:OD1	5:F:470:LYS:NZ	2.49	0.46
1:A:62:GLU:OE1	1:A:62:GLU:N	2.39	0.45
1:A:85:VAL:HG12	1:A:118:VAL:HG22	1.97	0.45
3:D:502:PRO:CB	8:P:15:DG:H22	2.30	0.45
5:F:280:GLU:HA	5:F:283:LEU:HG	1.96	0.45
6:M:27:GLU:OE1	6:M:27:GLU:N	2.48	0.45
2:C:932:VAL:HG13	2:C:935:LEU:HD22	1.98	0.45
2:C:1095:GLU:OE2	2:C:1095:GLU:HA	2.17	0.45
1:A:221:LEU:O	1:A:225:LEU:HD13	2.15	0.45
2:C:176:ASP:OD1	2:C:177:SER:N	2.49	0.45
2:C:938:GLU:OE2	2:C:942:ARG:NE	2.50	0.45
4:E:60:ASP:OD1	4:E:60:ASP:N	2.48	0.45
2:C:648:ASN:ND2	2:C:650:ASP:OD2	2.46	0.45
3:D:93:GLY:C	3:D:319:VAL:HG22	2.37	0.45
3:D:116:TYR:HB2	3:D:295:ARG:HG2	1.99	0.45
3:D:293:LEU:HG	3:D:1159:LEU:HD12	1.98	0.45
3:D:894:LEU:HD13	3:D:956:THR:OG1	2.17	0.45
2:C:776:ILE:HG21	2:C:788:LEU:CD1	2.46	0.45
3:D:320:ILE:O	3:D:325:ARG:NH2	2.49	0.45
1:B:203:ARG:HD3	1:B:205:ARG:HE	1.83	0.45
5:F:492:LYS:O	5:F:495:SER:OG	2.23	0.45
3:D:180:ASP:OD1	3:D:181:LEU:N	2.49	0.44
5:F:428:VAL:O	5:F:428:VAL:HG23	2.17	0.44
6:M:36:HIS:HA	6:M:39:LEU:HG	1.98	0.44
2:C:86:ASP:OD1	2:C:89:GLY:N	2.50	0.44
2:C:173:VAL:HG23	2:C:307:LYS:HG2	1.99	0.44
3:D:58:TRP:CE3	3:D:68:VAL:HG22	2.52	0.44
2:C:1116:LEU:HD21	3:D:402:LEU:HD12	2.00	0.44
3:D:20:ILE:HD13	3:D:316:CYS:O	2.17	0.44
3:D:170:LEU:HD12	3:D:173:ARG:NH2	2.33	0.44
5:F:466:ASP:OD2	5:F:468:GLN:NE2	2.50	0.44
1:A:176:TYR:HB2	1:A:192:LEU:HD11	1.98	0.44
3:D:356:ARG:NE	3:D:356:ARG:O	2.50	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:583:LEU:HD21	3:D:724:VAL:HG11	1.99	0.44
3:D:915:VAL:HG23	3:D:956:THR:HG21	1.99	0.44
2:C:155:VAL:HG22	2:C:160:GLU:OE2	2.17	0.44
3:D:663:LEU:O	3:D:667:LEU:HD23	2.18	0.44
3:D:1074:ILE:HD12	3:D:1078:ALA:HB2	2.00	0.44
3:D:67:ARG:HD3	3:D:67:ARG:HA	1.86	0.44
2:C:974:LEU:HD22	2:C:989:PRO:HA	2.00	0.44
5:F:472:LEU:HD13	5:F:487:ARG:HB2	2.00	0.44
2:C:1104:GLU:OE2	2:C:1105:SER:OG	2.36	0.43
3:D:1051:GLU:N	3:D:1051:GLU:OE1	2.51	0.43
5:F:284:ARG:O	5:F:287:VAL:HG12	2.18	0.43
1:A:29:GLY:O	1:B:40:ARG:NH1	2.49	0.43
2:C:130:ASN:OD1	2:C:131:GLU:N	2.51	0.43
3:D:353:ARG:O	3:D:357:LEU:HD23	2.18	0.43
2:C:210:VAL:HG12	2:C:249:THR:HG21	1.99	0.43
3:D:337:THR:HG23	3:D:341:ASN:HD22	1.84	0.43
3:D:468:ASN:O	3:D:471:SER:OG	2.29	0.43
5:F:486:ILE:HD12	5:F:489:ILE:HD11	2.00	0.43
3:D:920:LEU:CG	3:D:938:LEU:HD21	2.44	0.43
6:M:48:LEU:O	6:M:51:VAL:HG22	2.19	0.43
3:D:155:VAL:HG21	3:D:223:TRP:CH2	2.54	0.43
6:M:122:HIS:HA	6:N:126:ILE:HG22	1.99	0.43
2:C:37:LEU:O	2:C:439:ARG:NE	2.52	0.43
1:B:16:GLU:OE1	1:B:16:GLU:N	2.44	0.43
3:D:151:LEU:HD13	3:D:223:TRP:HH2	1.83	0.43
3:D:583:LEU:HD11	3:D:724:VAL:HG11	2.01	0.43
1:B:5:GLN:OE1	1:B:183:VAL:HG11	2.19	0.43
2:C:943:LEU:O	2:C:947:GLY:N	2.51	0.43
3:D:592:SER:OG	3:D:593:GLU:N	2.52	0.43
3:D:999:GLU:HG3	3:D:1000:PRO:HD3	2.01	0.43
2:C:171:PRO:HB2	2:C:300:GLY:HA3	2.00	0.43
2:C:574:SER:OG	2:C:575:VAL:N	2.52	0.43
2:C:627:VAL:CG2	2:C:687:VAL:HG13	2.49	0.43
2:C:1097:ILE:HD13	3:D:548:SER:HA	2.01	0.43
3:D:911:VAL:HG22	3:D:915:VAL:HG12	2.01	0.43
3:D:1206:ALA:HB3	3:D:1215:VAL:HG21	2.00	0.43
8:P:60:DC:C2'	8:P:61:DT:H72	2.49	0.43
2:C:690:ASP:OD2	2:C:696:ASN:N	2.49	0.42
3:D:959:ILE:HD11	3:D:968:THR:HG21	2.00	0.42
3:D:296:LEU:HD23	3:D:296:LEU:HA	1.91	0.42
3:D:621:LEU:HD11	3:D:664:GLY:CA	2.49	0.42



	i de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:F:240:ILE:HD12	5:F:275:LYS:HD3	2.01	0.42
3:D:1158:LEU:H	3:D:1158:LEU:HD23	1.85	0.42
2:C:174:TYR:HE1	2:C:303:LYS:HE3	1.83	0.42
3:D:763:GLU:OE2	3:D:767:GLN:NE2	2.52	0.42
4:E:17:ASP:OD1	4:E:18:GLU:N	2.51	0.42
2:C:276:THR:HB	2:C:279:ALA:HB3	2.02	0.42
3:D:738:LYS:O	3:D:741:VAL:HG12	2.19	0.42
5:F:360:ASN:OD1	5:F:361:LYS:N	2.53	0.42
5:F:473:ASP:OD2	8:P:47:DG:OP2	2.37	0.42
2:C:1030:SER:OG	2:C:1031:THR:N	2.53	0.42
6:M:11:ARG:O	6:M:16:ARG:NH2	2.53	0.42
1:B:211:ALA:O	1:B:214:THR:OG1	2.29	0.42
2:C:245:SER:O	2:C:249:THR:HG23	2.20	0.42
2:C:333:LYS:HE2	2:C:341:THR:HG21	2.01	0.42
2:C:604:LEU:HD23	2:C:604:LEU:H	1.85	0.42
1:A:97:LEU:HB2	1:A:110:ILE:HG13	2.01	0.42
5:F:432:ASP:O	5:F:435:SER:OG	2.26	0.42
2:C:120:PRO:O	2:C:121:LEU:HD22	2.19	0.42
3:D:671:LEU:HD23	3:D:711:LEU:HA	2.00	0.42
3:D:868:LEU:O	3:D:872:LEU:HD23	2.20	0.42
1:A:54:ILE:HD11	1:A:162:ILE:HD11	2.02	0.41
3:D:846:ILE:O	3:D:849:HIS:HB2	2.20	0.41
3:D:1121:VAL:HG11	3:D:1137:ILE:HD12	2.02	0.41
7:O:71:DG:H2'	7:O:71:DG:N3	2.34	0.41
2:C:1116:LEU:CD2	3:D:402:LEU:HD12	2.50	0.41
2:C:1106:PHE:HZ	3:D:10:LEU:HD21	1.85	0.41
3:D:810:ARG:O	3:D:814:GLY:N	2.53	0.41
6:M:52:TYR:O	6:M:55:LEU:HG	2.21	0.41
6:N:35:LEU:HD12	6:N:38:MET:CE	2.50	0.41
1:A:172:LEU:HD21	1:A:199:LYS:HG2	2.01	0.41
2:C:757:ARG:NH2	2:C:768:ALA:O	2.53	0.41
5:F:362:LEU:HA	5:F:365:VAL:HG22	2.02	0.41
2:C:52:ASP:OD1	2:C:53:ALA:N	2.54	0.41
2:C:644:ILE:HG22	2:C:658:LEU:HD11	2.02	0.41
2:C:518:THR:OG1	2:C:519:ALA:N	2.53	0.41
3:D:846:ILE:HD12	3:D:846:ILE:HA	1.85	0.41
3:D:102:THR:HG21	3:D:129:ILE:HD13	2.01	0.41
2:C:880:VAL:HG23	3:D:537:ASP:O	2.21	0.41
3:D:184:LEU:HD22	3:D:197:VAL:HB	2.02	0.41
3:D:288:LYS:HB3	3:D:288:LYS:HE3	1.78	0.41
3:D:751:VAL:HG11	3:D:768:GLU:CD	2.42	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:768:GLU:OE2	3:D:769:LEU:HG	2.21	0.41
7:O:15:DA:N6	8:P:69:DG:O6	2.54	0.41
8:P:21:DG:H2'	8:P:22:DG:H8	1.84	0.41
1:A:167:ILE:HG13	1:A:167:ILE:O	2.21	0.41
1:B:42:LEU:HD21	1:B:171:VAL:HG11	2.03	0.41
3:D:578:THR:HG21	3:D:685:LYS:HD3	2.03	0.41
3:D:821:ASN:HD22	3:D:821:ASN:HA	1.63	0.41
5:F:230:ALA:HA	5:F:233:GLU:OE2	2.21	0.41
6:N:35:LEU:HD12	6:N:38:MET:HE1	2.03	0.41
1:B:5:GLN:CD	1:B:183:VAL:HG11	2.42	0.40
2:C:67:ASP:OD1	2:C:68:VAL:N	2.54	0.40
2:C:1060:ALA:HB3	3:D:509:ILE:HD13	2.03	0.40
3:D:353:ARG:NH1	5:F:302:ASP:OD1	2.54	0.40
2:C:676:VAL:HG21	2:C:688:LEU:HD13	2.02	0.40
3:D:255:SER:OG	3:D:256:MET:N	2.54	0.40
3:D:619:LEU:HD21	3:D:663:LEU:HD13	2.03	0.40
3:D:93:GLY:O	3:D:319:VAL:HG22	2.22	0.40
8:P:23:DT:H2'	8:P:24:DC:C2	2.57	0.40
1:B:187:THR:O	1:B:187:THR:HG22	2.22	0.40
3:D:184:LEU:HD22	3:D:197:VAL:CG1	2.51	0.40
3:D:305:THR:HG22	3:D:1223:ALA:HB3	2.03	0.40
3:D:868:LEU:HD22	3:D:1023:LEU:HD11	2.03	0.40
3:D:1030:PHE:CE1	3:D:1140:ILE:HG21	2.56	0.40
3:D:1048:VAL:O	3:D:1085:GLY:CA	2.70	0.40
3:D:1081:LEU:H	3:D:1081:LEU:HD23	1.87	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	Perce	ntiles
1	А	224/340~(66%)	215~(96%)	9~(4%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	231/340~(68%)	224 (97%)	7 (3%)	0	100	100
2	С	$1114/1161 \ (96\%)$	1064 (96%)	50 (4%)	0	100	100
3	D	1257/1307~(96%)	1207~(96%)	49 (4%)	1 (0%)	51	85
4	Е	75/90~(83%)	74 (99%)	1 (1%)	0	100	100
5	F	299/531~(56%)	292~(98%)	7(2%)	0	100	100
6	М	129/159~(81%)	127~(98%)	2(2%)	0	100	100
6	Ν	129/159~(81%)	128 (99%)	1 (1%)	0	100	100
All	All	3458/4087~(85%)	3331 (96%)	126 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	132	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	194/279~(70%)	186~(96%)	8 (4%)	30	56
1	В	199/279~(71%)	197~(99%)	2(1%)	76	86
2	С	942/979~(96%)	933~(99%)	9(1%)	76	86
3	D	1054/1095~(96%)	1044 (99%)	10 (1%)	78	88
4	Ε	64/74~(86%)	64 (100%)	0	100	100
5	F	258/430~(60%)	257~(100%)	1 (0%)	91	94
6	М	99/120~(82%)	99 (100%)	0	100	100
6	Ν	99/120~(82%)	$98 \ (99\%)$	1 (1%)	76	86
All	All	2909/3376~(86%)	2878 (99%)	31 (1%)	74	84

All (31) residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
1	А	36	ASN
1	А	81	LYS
1	А	106	THR
1	А	110	ILE
1	А	131	LYS
1	А	152	ASN
1	А	182	ARG
1	А	223	ARG
1	В	55	ARG
1	В	150	VAL
2	С	153	THR
2	С	173	VAL
2	С	466	TYR
2	С	639	VAL
2	С	743	VAL
2	С	856	ARG
2	С	1036	MET
2	С	1038	THR
2	С	1109	LEU
3	D	247	ARG
3	D	287	GLN
3	D	712	LYS
3	D	762	LYS
3	D	819	VAL
3	D	821	ASN
3	D	842	LEU
3	D	1093	LYS
3	D	1209	PHE
3	D	1210	GLN
5	F	502	ARG
6	N	16	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such side chains are listed below:

Mol	Chain	Res	Type
1	А	36	ASN
3	D	103	HIS
3	D	287	GLN
3	D	525	HIS
3	D	821	ASN
5	F	282	ASN
5	F	499	HIS



5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	4/5~(80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	Q	5	G

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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-32077. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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

6.2.2 Raw 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: 204



Y Index: 171



Z Index: 179

6.3.2 Raw map



X Index: 204

Y Index: 171



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



6.4.2 Raw map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



Mask visualisation (i) 6.6

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

emd_32077_msk_1.map (i) 6.6.1







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 770 $\rm nm^3;$ this corresponds to an approximate mass of 695 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 (i)



*Reported resolution corresponds to spatial frequency of 0.242 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.242 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	4.14	-	-	
Author-provided FSC curve	4.14	6.46	4.20	
Unmasked-calculated*	7.43	14.99	7.95	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.43 differs from the reported value 4.14 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32077 and PDB model 7VPZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.05 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 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 (0.05).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9670	0.2620	1.0
А	0.9770	0.2750	
В	0.9800	0.2360	
С	0.9830	0.3180	
D	0.9780	0.3000	
E	0.9490	0.2760	
F	0.9710	0.2160	
М	0.7750	0.0390	
N	0.9020	0.0610	
0	0.9600	0.1780	0.0 <
Р	0.9530	0.1570	
Q	0.9540	0.2760	

