



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:30 PM UTC

PDB ID : 8F5O / pdb_00008f5o
EMDB ID : EMD-28866
Title : Structure of Leishmania tarentolae IFT-A (state 1)
Authors : Zhou, H.; Brown, A.
Deposited on : 2022-11-14
Resolution : 3.50 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
MolProbity : 4-5-2 with Phenix2.0
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

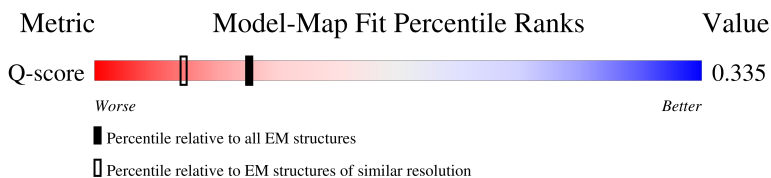
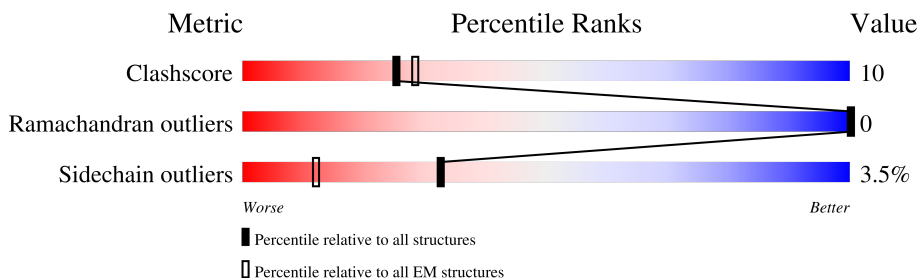
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	B	1247	
2	C	1292	
3	E	1654	
4	A	368	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	1376	31% 54% 12% 34%
6	D	1642	47% 23% 28%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43398 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 Intraflagellar transport protein 122B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1134	Total	C	N	O	S	0	0
			8965	5674	1570	1658	63		

- Molecule 2 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1179	Total	C	N	O	S	0	0
			9354	5929	1622	1735	68		

- Molecule 3 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1076	Total	C	N	O	S	0	0
			8380	5291	1451	1588	50		

- Molecule 4 is a protein called NET domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	53	Total	C	N	O	S	0	0
			427	264	69	87	7		

- Molecule 5 is a protein called WD_REPEATS_REGION domain-containing protein.

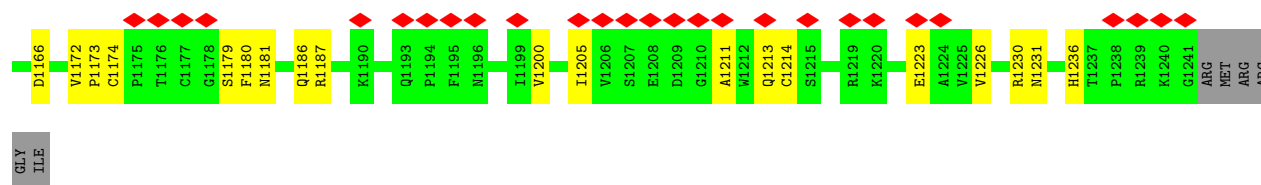
Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	911	Total	C	N	O	S	0	0
			7045	4431	1231	1349	34		

- Molecule 6 is a protein called TPR_REGION domain-containing protein.

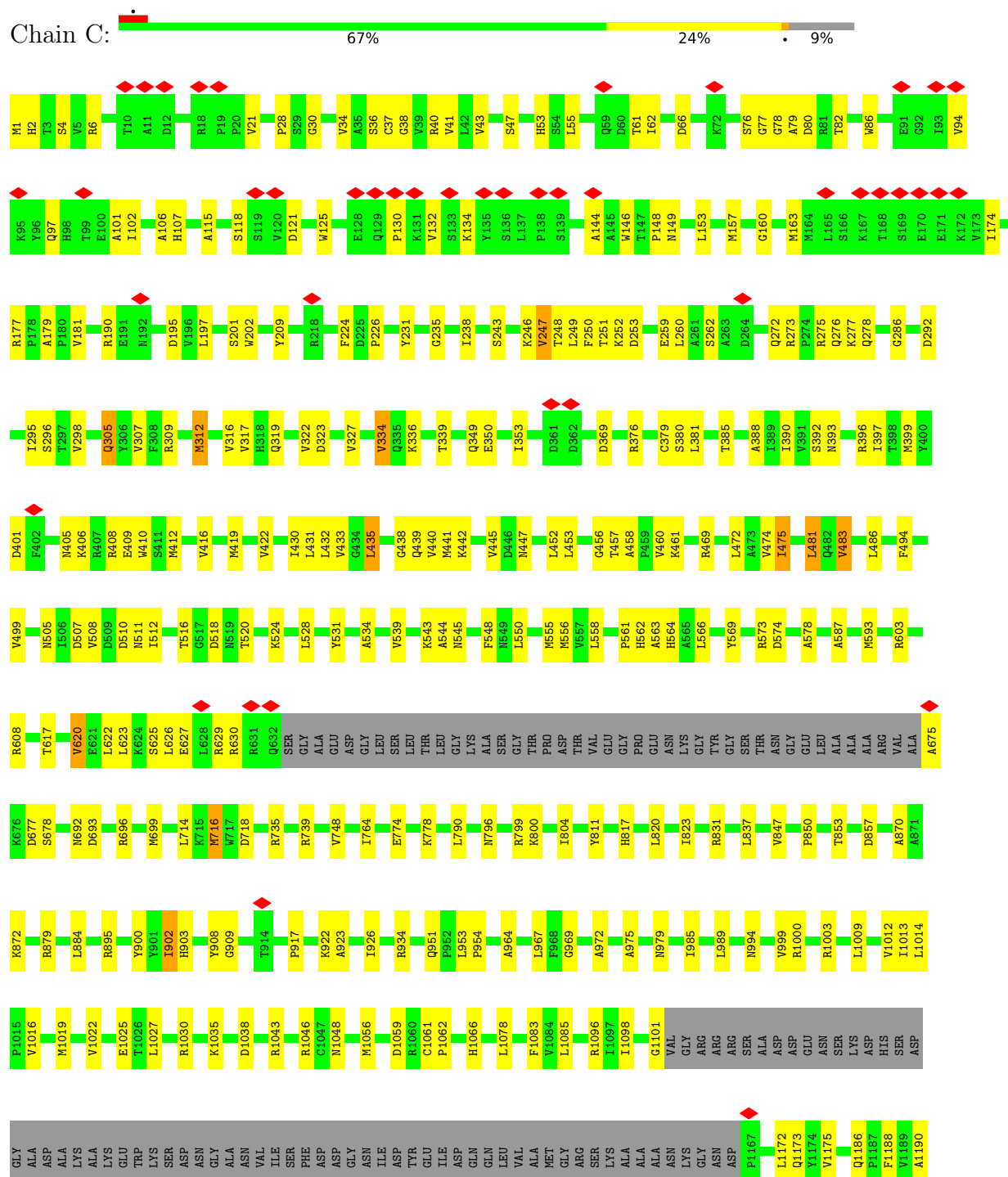
Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1180	Total	C	N	O	S	0	0
			9223	5796	1638	1738	51		

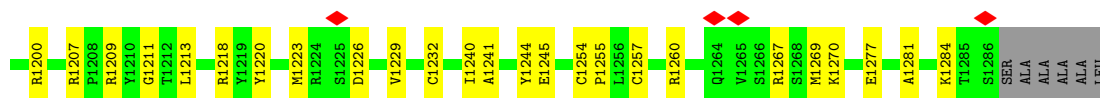
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	B	2	Total 2	Zn 2	0
7	C	2	Total 2	Zn 2	0

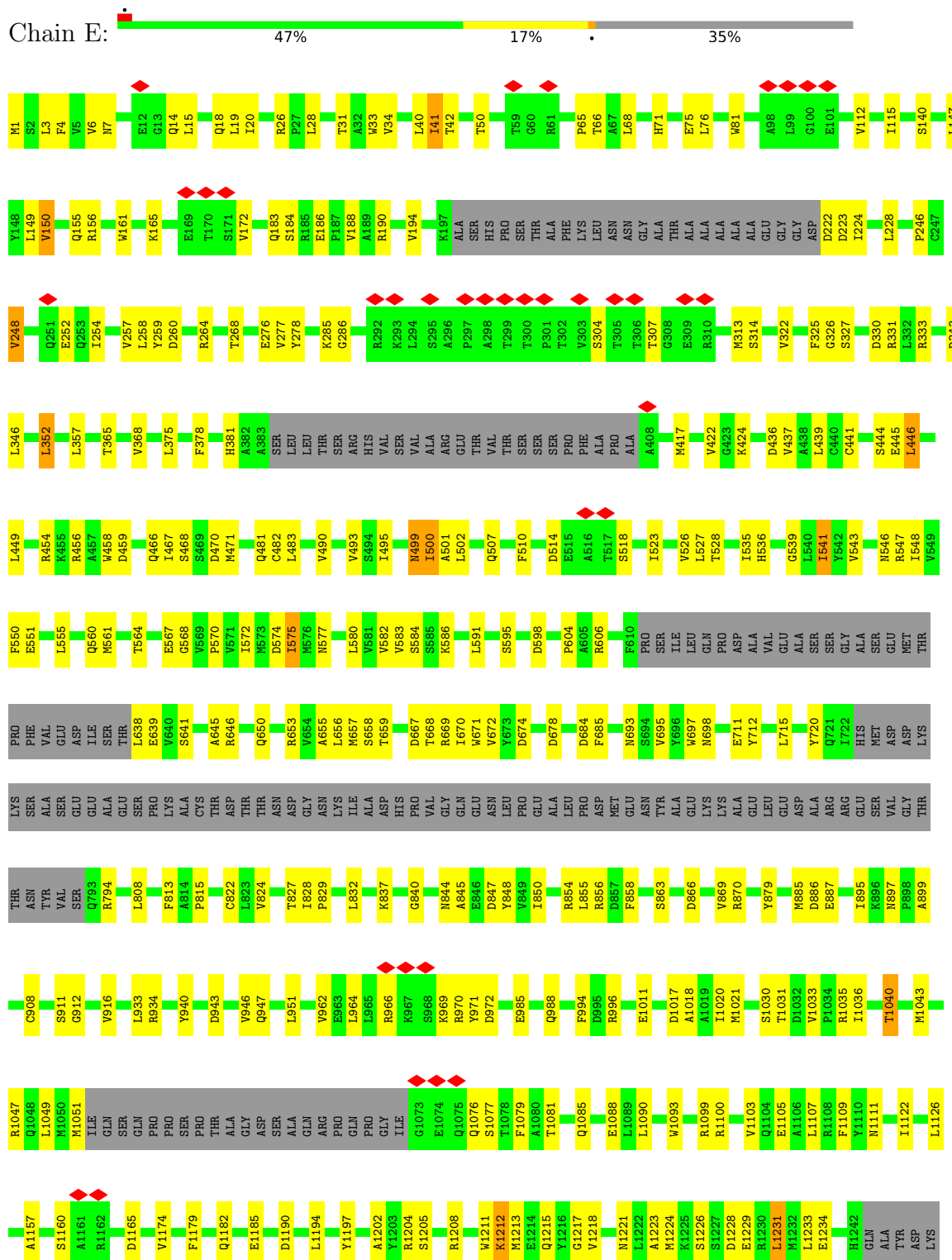


• Molecule 2: Intraflagellar transport protein 122 homolog





• Molecule 3: WD_REPEATS_REGION domain-containing protein



GLN	ASP	GLU	ILE	TRP	VAL	ALA
ASN	HIS	GLU	LYS	SER	GLU	GLN
ALA	SER	LYS	SER	ALA	MET	VAL
LYS	LEU	VAL	ILE	CYS	LEU	LEU
SER	ILE	GLU	VAL	LYS	PHE	ARG
LEU	GLN	GLN	LEU	ALA	ALA	ARG
ALA	ASP	LEU	PHE	LYS	ILE	GLY
ASN	LEU	LYS	THR	THR	HIS	GLY
VAL	LEU	GLN	THR	GLN	PHE	ALA
LEU	ARG	ARG	LYS	ALA	GLU	GLN
PRO	ILE	VAL	ALA	GLY	GLU	GLN
GLY	GLY	GLU	LYS	ASP	ALA	CYS
GLY	ASP	ILE	ALA	ARG	LEU	ALA
ILE	VAL	LEU	TRP	VAL	LEU	ALA
ALA	PHE	LYS	MET	LYS	LEU	ASP
THR	ALA	ALA	ASN	ALA	CYS	ALA
GLU	LEU	PHE	LEU	MET	GLU	CYS
ALA	MET	VAL	LEU	ARG	THR	VAL
PRO	VAL	LYS	ALA	MET	GLN	GLN
GLY	ARG	ALA	PHE	LEU	ASN	GLY
ALA	PHE	GLN	THR	MET	ALA	GLY
VAL	TYR	LYS	GLU	ARG	THR	LEU
TRP	PHE	THR	SER	GLY	LEU	TYR
GLU	ASP	VAL	CYS	GLY	THR	GLU
GLY	LYS	ASP	ALA	GLU	GLU	THR
ALA	LEU	SER	GLN	LYS	LEU	LEU
ARG	GLY	MET	LEU	GLU	MET	HIS
LYS	GLU	VAL	HIS	VAL	ALA	GLU
PHE	PRO	VAL	ILE	VAL	GLU	VAL
SER	HIS	ALA	ASP	ILE	SER	SER
THR	ASN	GLU	GLU	PHE	MET	ALA
ASP	LEU	ARG	ASN	THR	THR	ALA
THR	ALA	GLY	ARG	ALA	SER	PHE
ARG	LYS	SER	ASN	ASN	ASN	ALA
ARG	VAL	VAL	TYR	HIS	ILE	SER
SER	MET	ALA	PRO	SER	GLY	GLY
SER	GLU	GLU	GLU	ARG	LEU	SER
VAL	SER	VAL	ALA	LYS	LEU	THR
ILE	ILE	MET	ALA	VAL	SER	ASP
PRO	MET	LYS	ARG	GLU	MET	PRO
ASP	LYS	ALA	ALA	ILE	GLU	ALA
GLU	HIS	ASP	LEU	ILE	GLU	VAL
VAL	GLY	SER	GLU	THR	ARG	PHE
ARG	ALA	VAL	ASP	MET	GLN	GLY
VAL	ASP	ILE	CYS	ALA	ALA	LEU
VAL	PRO	CYS	ILE	ASN	VAL	MET
	GLN	ALA	ALA	ALA	LEU	ALA
	LEU	CYS	ALA	PHE	ARG	ASP
	PHE	SER	GLU	LEU	ARG	ASP
	ILE	GLY	GLU	GLN	VAL	HIS
	ALA	ILE	VAL	GLN	ALA	SER
	ASP	LYS	ARG	ASN	ILE	GLU
	TYR	GLY	GLY	THR	ALA	SER
	MET	ARG	LYS	SER	VAL	ASP
	GLU	ARG	LYS	ALA	GLN	TYR
	ARG	PRO	ALA	ASP	GLN	GLN
	VAL	SER	ASN	ASN	GLY	LYS
	CYS	SER	ILE	ALA	ARG	ALA

- Molecule 4: NET domain-containing protein

Chain A: 10% 86%

[illegible]

- Molecule 5: WD_REPEATS_REGION domain-containing protein

Chain F: 31% 54% 12% 34%

M1	V2	L3	T4	Q5	D6	F7	V8	I9	S10	M11	A12	D13	L14	G15	A16	G17	H18	V19	Y20	E21	A22	L23	H24	P25	S26	S27	P28	L29	I30	A31	L32	A33	G34	S35	K36	G37	K38	V39	L40	T41	L42	M43	K44	T45	G46	K47	V48	E49	H50	Q51	L52	P53	M54	S55	N56	V57	V58	A59	W60
E61	W62	E63	C64	S65	T66	D67	T68	L69	A70	I71	I72	T73	S74	S75	S76	S77	D78	V79	H80	L81	Y82	T83	H84	R85	T86	R87	Q88	T89	D90	T91	I92	D93	T94	K95	L96	K97	D98	L99	C100	F101	W102	C103	W104	S105	Q106	S107	Q108	P109	L110	F111	A112	I113	G114	S115	K116	S117	G118	Q119	W120

ALA	VAL	PRO	THR	ASP	SER	ALA	Q769	V637	L502	F389	D301	F241	V181	V121
VAL	ASP	LYS	LEU	SER	ASN	ALA	W770	L651	T505	L390	G302	L242	P182	L122
PRO	THR	THR	GLU	THR	GLN	VAL	R772	L651	T505	A399	I303	A243	K183	Y123
THR	THR	THR	ALA	ASP	ASP	ALA	E784	N655	V511	V401	A304	G244	S184	N124
PRO	THR	THR	GLU	THR	THR	LYS	W785	N656	L514	Q404	P305	F245	V185	R125
MET	THR	THR	THR	THR	THR	LYS	I786	L659	T522	E409	T306	A246	C186	R126
VAL	THR	THR	THR	THR	THR	LYS	F787	R660	T522	E409	D308	S247	S188	T127
THR	THR	THR	THR	THR	THR	LYS	I788	T661	R531	E409	E309	T249	G189	L128
THR	THR	THR	THR	THR	THR	LYS	S789	E665	R531	E409	E309	V250	M190	L130
THR	THR	THR	THR	THR	THR	LYS	Q794	L673	A532	I412	A310	A251	A191	V131
THR	THR	THR	THR	THR	THR	LYS	H795	L673	F533	P80	S311	L252	N192	P132
THR	THR	THR	THR	THR	THR	LYS	L796	R677	A534	ASN	L312	L253	M192	V133
THR	THR	THR	THR	THR	THR	LYS	E797	R677	N535	SER	E314	D254	P194	A134
THR	THR	THR	THR	THR	THR	LYS	R798	R677	T539	LEU	P194	L255	K195	D135
THR	THR	THR	THR	THR	THR	LYS	R799	S679	T539	PRO	E315	A256	S196	T136
THR	THR	THR	THR	THR	THR	LYS	G800	N681	V556	TYR	R316	A256	S197	H137
THR	THR	THR	THR	THR	THR	LYS	W801	N681	Q570	PRO	G317	A256	S197	K138
THR	THR	THR	THR	THR	THR	LYS	Y802	N681	K571	VAL	P319	A256	S197	Q139
THR	THR	THR	THR	THR	THR	LYS	A805	Q687	N572	ASP	D320	V260	A200	R140
THR	THR	THR	THR	THR	THR	LYS	E807	Q687	L574	ALA	L321	R261	V202	L141
THR	THR	THR	THR	THR	THR	LYS	R803	E690	V582	VAL	L322	L262	V202	I142
THR	THR	THR	THR	THR	THR	LYS	R814	E690	T585	SER	A323	R263	N203	S143
THR	THR	THR	THR	THR	THR	LYS	S822	I706	V586	SER	W324	G264	L204	G144
THR	THR	THR	THR	THR	THR	LYS	S826	R707	D587	GLN	S325	S265	D205	M145
THR	THR	THR	THR	THR	THR	LYS	V827	V718	F594	GLN	R326	L266	N206	W146
THR	THR	THR	THR	THR	THR	LYS	E833	V718	V595	A434	Q329	R267	N207	V147
THR	THR	THR	THR	THR	THR	LYS	E837	L721	H599	L439	L331	L268	T207	P148
THR	THR	THR	THR	THR	THR	LYS	Q838	L721	S600	E443	F332	L269	L209	A149
THR	THR	THR	THR	THR	THR	LYS	C839	L723	S608	S446	I210	K270	I210	Q150
THR	THR	THR	THR	THR	THR	LYS	R840	R725	V611	S446	V211	N271	D151	D151
THR	THR	THR	THR	THR	THR	LYS	Q841	R725	V611	S446	D212	V273	S152	S152
THR	THR	THR	THR	THR	THR	LYS	G842	E729	V611	S446	D213	E274	R214	R153
THR	THR	THR	THR	THR	THR	LYS	A843	K730	D613	V460	L213	M275	S215	L154
THR	THR	THR	THR	THR	THR	LYS	A844	K730	S614	V461	R214	V276	Y216	L155
THR	THR	THR	THR	THR	THR	LYS	R845	L732	D617	Y462	S215	N277	I157	I156
THR	THR	THR	THR	THR	THR	LYS	R846	L734	N618	V466	Y216	F278	A217	I157
THR	THR	THR	THR	THR	THR	LYS	S846	K745	L619	V466	T218	G279	S158	S158
THR	THR	THR	THR	THR	THR	LYS	Q847	K745	V620	S469	A219	E280	E159	E159
THR	THR	THR	THR	THR	THR	LYS	T848	N749	T621	S469	A220	G281	D160	D160
THR	THR	THR	THR	THR	THR	LYS	R849	S754	P622	D473	G221	S282	P161	P161
THR	THR	THR	THR	THR	THR	LYS	T850	S755	L623	P480	Q221	G283	S162	S162
THR	THR	THR	THR	THR	THR	LYS	Q851	Q756	P624	P480	Q222	G283	L163	L163
THR	THR	THR	THR	THR	THR	LYS	H852	R764	P629	D488	F223	V284	I164	I164
THR	THR	THR	THR	THR	THR	LYS	T853	R764	P629	D488	N224	V284	I165	I165
THR	THR	THR	THR	THR	THR	LYS	A854	R766	P633	L491	S225	V285	S166	S166
THR	THR	THR	THR	THR	THR	LYS	D855	R766	P633	L491	A226	A286	D167	D167
THR	THR	THR	THR	THR	THR	LYS	D856	R766	P633	L491	L227	V288	A168	A168
THR	THR	THR	THR	THR	THR	LYS	A856	R766	P633	L491	G228	V288	E169	E169
THR	THR	THR	THR	THR	THR	LYS	H857	R766	P633	L491	Q229	V288	G170	G170
THR	THR	THR	THR	THR	THR	LYS	K858	R766	P633	L491	I230	V288	K171	K171
THR	THR	THR	THR	THR	THR	LYS	T859	R766	P633	L491	I231	V288	V172	V172
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	C232	V288	L173	L173
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	L233	V288	T174	T174
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	A235	V288	T175	T175
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	G236	V288	I176	I176
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	I237	V288	P177	P177
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	N238	V288	L178	L178
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	G239	V288	P179	P179
THR	THR	THR	THR	THR	THR	LYS	H860	R766	P633	L491	E240	V288	S180	S180

ALA
LEU
MET
THR
ARG
LEU
SER
GLY
THR
THR
THR
CYS
PRO
MET
CYS
GLU
ALA
THR
THR
ASP
ILE
ILE
SER
ASN
VAL
ASN
ARG
GLU
THR
THR
LEU
LEU
ALA
LEU

• Molecule 6: TPR_REGION domain-containing protein

Chain D:



MET
GLN
PRO
SER
SER
PHE
LEU
PRO
PRO
ASP
VAL
TRP
MET
ALA
VAL
THR
LEU
THR
ASN
ALA
GLU
PRO
HIS
ILE
ILE
PRO
GLU
ILE
THR
THR
PRO
LEU
SER
THR
ASN
PRO
GLU
LEU
ALA
ALA
PHE
ILE
SER
THR
VAL
ARG
GLY
CYS
LEU
SER
LYS
VAL
LYS
LYS
GLN
ARG
THR
ALA
ASP
PRO
PRO
PRO

SER
PRO
PRO
ARG
VAL
TRP
SER
SER
ALA
LEU
PRO
C322
THR
LEU
GLY
GLU
TRP
ARG
GLN
GLY
MET
ALA
ALA
ASN
ASP
ASP
ALA
ALA
ILE
ARG
MET
GLU
THR
GLY
TYR
LYS
THR
ILE
VAL
ASN
ALA
GLU
SER
TYR
PHE
GLN
ASP
ARG
ILE
THR
LEU
ALA
LEU
LEU
LEU
PHE
THR
ASP
MET
GLY
ARG
GLU
SER
GLY
THR
THR
LYS
TRP
HIS
ALA
GLU
ASP
GLU
VAL
THR
CYS
LEU
SER
LYS
VAL
ILE
ALA
GLN
GLN
THR
SER
THR
ALA
ASP
HIS

MET
PHE
ARG
VAL
TRP
ARG
SER
ALA
LEU
THR
C322
THR
LEU
GLY
GLU
TRP
ARG
GLN
GLY
MET
ALA
ALA
ASN
ASP
ASP
ALA
ALA
ILE
ARG
MET
GLU
THR
GLY
TYR
LYS
THR
ILE
VAL
ASN
ALA
GLU
SER
TYR
PHE
GLN
ASP
ARG
ILE
THR
LEU
ALA
LEU
LEU
LEU
PHE
THR
ASP
MET
GLY
ARG
GLU
SER
GLY
THR
THR
LYS
TRP
HIS
ALA
GLU
ASP
GLU
VAL
THR
CYS
LEU
SER
LYS
VAL
ILE
ALA
GLN
GLN
THR
SER
THR
ALA
ASP
HIS

ASP
GLY
PHE
GLU
ILE
ALA
ALA
ASN
MET
MET
GLY
GLU
TRP
ARG
GLN
VAL
ALA
VAL
GLN
ALA
PHE
THR
LEU
THR
ASN
GLY
TYR
GLY
THR
THR
LYS
TRP
HIS
ALA
GLU
ASP
GLU
TYR
THR
ASN
GLN
TYR
GLY
THR
THR
LYS
VAL
ILE
ALA
GLN
GLN
THR
TRP
GLY
ASP
LEU
LEU

LEU
SER
GLY
ARG
GLY
ALA
LEU
LEU
LEU
LYS
C321
GLY
ALA
GLY
TRP
ARG
GLN
VAL
PHE
THR
PHE
SER
VAL
VAL
ASP
MET
ASP
MET
GLU
GLU
GLU
ALA
GLN
ILE
ASN
VAL
TYR
SER
TYR
PHE
GLN
ASP
ARG
ILE
THR
LEU
ASN
GLY
SER
SER
ARG
GLY
THR
THR
LYS
TRP
ILE
ASP
LEU
ASN
ASP
ALA
ALA
L291
L292
V295
L304
K305
K306
A307

L311
D312
F315
F319
N320
S322
I323
P324
P325
L326
V327
P328
P329
R330
R331
L332
M334
Q335
D338
W339
S354
S355
N356
P357
E358
A361
L362
E363
A367
M368
A369
K370
D371
T372
R373
H374
D375
A376
A377
R380
R383
R389
L389
H400
Q401
F402
A403
L404

V405
R408
A410
R413
D415
Q422
R433
L438
C439
G440
L441
Q442
Q445
L446
Y447
R448
D451
K452
T455
E456
R459
D469
T474
V475
Q481
A487
L493
Q498
P499
A500
A501
E506
L507
S508
M509
L510
N511
R515
W516
R519

G520
E523
T524
A526
V527
L528
R529
Y530
L531
D532
Q533
A534
E535
E536
A537
Q540
D541
V542
K543
E544
R545
A546
G547
V548
G549
M550
E551
V552
V554
H555
L556
N557
A558
A561
A567
I569
M570
H571
MET
PHE
LYS
HIS
ASP
V586
Y587
G588
G589
K590
R593

H594
L595
V599
Q600
H601
A604
C605
M606
E607
A608
Q609
L610
K614
W615
V616
F617
V618
T619
V622
T632
L633
Q636
P641
D642
A643
F644
L645
C651
D656
T657
L664
A665
Q666
T669
L670
D671
F672
L679
Y680
M681
L682
K688
GLY
THR
THR
GLY

TYR
ALA
GLU
ALA
LEU
ALA
SER
LEU
GLN
ARG
ALA
TYR
ASN
THR
VAL
LYS
S710
A717
GLY
LYS
PRO
THR
THR
ASN
PRO
LEU
SER
V726
Y733
Q738
A739
Q740
D745
A749
R750
E751
T752
L753
T754
E755
A756
L758
K759
F760
R761
Q765
I766
G767
R768
V769
I770
I771
A772
Q773

A777
D781
K784
S785
L788
L789
K795
F798
Y799
I800
A801
A802
H803
S804
Q805
L806
G807
K808
L811
T812
H813
R814
H815
F824
Q835
S836
E839
L840
G841
E842
A843
I847
Q848
E849
P850
E851
Q852
A853
I854
Y857
S867
L870
S871
V874

L878
D883
K886
Y890
Y891
Q892
D893
R905
A906
D907
I918
E923
V926
E932
LEU
PRO
SER
THR
ASP
GLY
ALA
GLY
ALA
VAL
ALA
SER
ALA
ALA
ALA
ALA
E953
A954
T957
E960
R961
N963
L964
Y965
L966
L967
L968
Y969
A1083
R1084
E1085
Y1086

R973
D974
Q975
P976
Y977
T978
V979
E983
N984
D997
A998
A999
L1000
T1001
A1002
L1003
T1005
S1008
L1009
Q1010
R1011
R1012
L1013
L1014
E1015
L1016
Q1017
L1018
E1029
Q1030
V1032
V1033
M1034
S1035
E1036
I1037
C1038
C1045
M1059
L1070
A1071
V1072
Q1073
T1081
M1082
A1083
R1084
E1085
Y1086

L1087	L1088	E1089	A1090	D1094	E1095	S1096	N1097	E1098	Q1106	Y1109	R1110	E1115	E1118	Q1119	T1122	T1123	R1126	M1127	A1135	I1139	L1140	L1141	L1144	Y1145	T1146	E1147	Q1148	R1149	R1150	A1154	R1155	N1156	M1157	F1158	E1159	D1160	L1161	L1162	R1163	K1164	T1165	H1168	Y1169	L1172	V1173				
H1181	K1189	E1193	R1194	A1197	A1198	Y1211	E1217	N1221	N1222	E1225	A1226	L1227	L1228	L1235	P1236	N1239	C1242	R1248	M1249	I1250	Y1253	T1257	T1258	Q1259	D1260	L1261	W1262	V1263	R1264	G1265	T1266	SER	PRO	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ASP	PRO	PRO	ARG			
ALA	LYS	GLN	GLN	LYS	SER	ASN	ALA	THR	GLY	PRO	GLY	LYS	VAL	PRO	LEU	LYS	ALA	ALA	T1301	T1302	L1307	H1308	D1309	N1310	I1311	R1312	L1317	L1318	L1319	P1322	V1323	E1327	A1333	T1336	M1337	A1338	T1339	R1340	R1341	P1342	L1345	F1352	L1353	E1354	C1355	I1356	T1361	GLY	VAL
SER	ALA	ALA	MET	THR	ALA	GLU	LYS	ASN	GLY	PRO	GLY	SER	GLY	SER	PRO	LYS	THR	ALA	ALA	GLU	GLU	ARG	GLN	PRO	ARG	ARG	GLY	LYS	GLY	GLY	ASP	SER	ASP	ASP	GLN	LEU	LEU	ALA	SER	MET	HIS	GLY	ALA	ALA	ALA	GLU	LEU	ALA	ASN
S1425	T1426	A1427	F1431	A1432	L1433	Q1434	V1437	T1438	H1439	P1440	F1443	L1446	T1452	Q1455	E1456	T1457	R1460	N1461	V1462	R1465	L1466	S1469	T1472	T1473	T1474	K1475	M1476	M1479	K1485	GLU	ASP	ALA	ALA	SER	LYS	ASP	ALA	ALA	ALA	SER	LYS	GLY	ALA	ALA	GLU	ALA	ALA		
PRO	MET	V1506	L1507	S1508	P1509	E1510	I1511	L1514	E1518	E1523	M1526	L1527	Y1531	M1532	D1533	T1534	Q1535	R1538	L1539	K1540	D1541	A1542	R1543	F1544	S1551	A1552	N1553	S1557	W1560	N1561	E1562	L1565	T1566	Y1567	K1572	H1573	K1574	W1575	A1576	S1577	Q1578	C1579	K1582	A1583	W1584	E1589			
A1590	D1591	P1592	D1593	V1594	K1597	N1601	Q1607	P1608	V1609	K1610	A1611	I1612	D1613	K1616	R1617	T1624	Y1625	P1626	R1627	I1628	M1633	D1634	Y1637	S1638	M1639	L1640	R1641	P1642																					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	239280	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 ($e^-/\text{\AA}^2$)	57.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	86.420	Depositor
Minimum map value	-36.983	Depositor
Average map value	0.020	Depositor
Map value standard deviation	1.359	Depositor
Recommended contour level	9	Depositor
Map size ($\text{\AA}$)	514.6, 514.6, 514.6	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	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

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	B	0.17	0/9156	0.33	0/12403
2	C	0.16	0/9548	0.34	0/12921
3	E	0.19	0/8546	0.35	0/11608
4	A	0.15	0/432	0.40	0/584
5	F	0.16	0/7173	0.31	0/9746
6	D	0.22	0/9377	0.41	0/12718
All	All	0.18	0/44232	0.35	0/59980

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	B	8965	0	8873	178	0
2	C	9354	0	9301	202	0
3	E	8380	0	8309	175	0
4	A	427	0	413	10	0
5	F	7045	0	7054	103	0
6	D	9223	0	9265	259	0
7	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	2	0	0	0	0
All	All	43398	0	43215	903	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 10.

All (903) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:441:CYS:O	3:E:445:GLU:HB3	1.71	0.89
5:F:446:SER:HB3	5:F:462:TYR:HB2	1.66	0.78
2:C:197:LEU:HB3	2:C:209:TYR:O	1.84	0.76
5:F:789:SER:HB3	5:F:808:MET:HB2	1.66	0.76
6:D:567:ALA:HA	6:D:570:MET:HE2	1.70	0.73
3:E:499:ASN:N	3:E:499:ASN:OD1	2.22	0.73
6:D:1034:MET:SD	6:D:1034:MET:N	2.60	0.72
6:D:682:LEU:HD11	6:D:738:GLN:HB3	1.71	0.72
3:E:570:PRO:HA	3:E:584:SER:HA	1.70	0.72
2:C:4:SER:HB3	2:C:292:ASP:O	1.90	0.71
6:D:569:ILE:HD13	6:D:614:LYS:HD2	1.73	0.71
1:B:462:ILE:HD13	1:B:514:LEU:HD21	1.74	0.69
1:B:116:ALA:HB3	1:B:125:CYS:HB3	1.73	0.69
3:E:514:ASP:O	3:E:518:SER:N	2.26	0.69
6:D:1236:PRO:O	6:D:1239:ASN:ND2	2.25	0.69
6:D:1010:GLN:NE2	6:D:1030:GLN:OE1	2.27	0.68
6:D:799:TYR:O	6:D:802:ALA:HB3	1.93	0.68
3:E:1208:ARG:O	3:E:1212:LYS:NZ	2.27	0.67
5:F:321:LEU:HB3	5:F:334:GLY:O	1.95	0.67
6:D:1308:HIS:HA	6:D:1311:ILE:HD12	1.76	0.67
1:B:353:TRP:HE1	1:B:358:ASN:HA	1.60	0.67
1:B:1063:ARG:HA	1:B:1149:ARG:HH12	1.60	0.66
1:B:266:THR:O	1:B:274:PRO:HA	1.96	0.66
1:B:846:VAL:HA	2:C:430:ILE:HD11	1.78	0.66
6:D:651:CYS:HB3	6:D:656:ASP:HB2	1.78	0.66
6:D:1135:ALA:HB2	6:D:1168:HIS:HE1	1.59	0.66
6:D:1123:THR:HA	6:D:1126:ARG:HE	1.60	0.65
5:F:23:LEU:HD13	5:F:326:ARG:HH22	1.61	0.65
6:D:1591:ASP:OD2	6:D:1594:VAL:N	2.27	0.65
1:B:118:ASN:ND2	1:B:120:SER:OG	2.30	0.65
2:C:442:LYS:HG3	2:C:453:LEU:HD11	1.79	0.65
2:C:336:LYS:NZ	2:C:379:CYS:SG	2.70	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:735:ARG:HG3	2:C:739:ARG:HH22	1.62	0.64
4:A:162:SER:OG	4:A:185:ARG:NH2	2.31	0.64
3:E:656:LEU:HB2	3:E:671:TRP:HB2	1.80	0.64
2:C:41:VAL:HB	2:C:55:LEU:HB2	1.80	0.64
6:D:803:HIS:HA	6:D:806:LEU:HB3	1.79	0.64
2:C:1078:LEU:HD21	2:C:1240:ILE:HG12	1.80	0.64
3:E:20:ILE:HG22	3:E:31:THR:HG22	1.78	0.64
2:C:272:GLN:NE2	2:C:276:GLN:O	2.32	0.63
3:E:454:ARG:NH2	3:E:822:CYS:SG	2.66	0.63
6:D:632:THR:O	6:D:636:GLN:NE2	2.32	0.63
2:C:524:LYS:NZ	2:C:528:LEU:O	2.30	0.63
3:E:454:ARG:O	3:E:456:ARG:NH1	2.31	0.63
2:C:505:ASN:HB2	2:C:511:ASN:HB2	1.81	0.63
2:C:902:ILE:HD13	2:C:1257:CYS:HB3	1.81	0.63
2:C:1056:MET:HE1	2:C:1062:PRO:HA	1.80	0.63
2:C:1000:ARG:O	2:C:1000:ARG:NH1	2.31	0.63
5:F:324:TRP:O	5:F:326:ARG:NH2	2.29	0.63
1:B:646:GLU:HB3	1:B:650:LEU:HB3	1.80	0.62
6:D:1443:PHE:HB3	6:D:1465:ARG:HH22	1.64	0.62
6:D:1032:VAL:O	6:D:1035:SER:OG	2.16	0.62
5:F:784:GLU:HG3	5:F:788:ILE:HD11	1.80	0.62
6:D:1263:VAL:O	6:D:1340:ARG:NH2	2.32	0.62
6:D:1475:LYS:NZ	6:D:1508:SER:O	2.33	0.62
5:F:266:LEU:HD21	5:F:303:ILE:HD12	1.82	0.62
5:F:364:ASN:OD1	5:F:365:ARG:NH1	2.32	0.62
1:B:254:ASN:ND2	1:B:256:SER:OG	2.33	0.62
3:E:26:ARG:HG3	3:E:75:GLU:HG2	1.82	0.62
5:F:223:PHE:HB3	5:F:227:LEU:HD12	1.82	0.62
2:C:1207:ARG:HB3	2:C:1209:ARG:HH21	1.65	0.61
2:C:1269:MET:SD	2:C:1269:MET:N	2.70	0.61
3:E:15:LEU:HD22	3:E:446:LEU:HB2	1.82	0.61
6:D:1466:LEU:O	6:D:1469:SER:OG	2.18	0.61
1:B:433:TRP:HE1	1:B:457:SER:HB2	1.66	0.61
3:E:972:ASP:OD1	3:E:972:ASP:N	2.34	0.61
6:D:536:GLU:O	6:D:540:GLN:NE2	2.33	0.61
1:B:200:LEU:HA	1:B:223:TYR:HA	1.83	0.61
5:F:122:LEU:HB2	5:F:131:VAL:HB	1.83	0.61
1:B:532:ASN:ND2	1:B:534:ASN:OD1	2.34	0.61
6:D:1159:GLU:O	6:D:1163:ARG:N	2.33	0.61
2:C:316:VAL:HG12	2:C:327:VAL:HG22	1.83	0.61
1:B:797:ALA:HB2	1:B:812:ILE:HG21	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:545:ASN:OD1	2:C:562:HIS:NE2	2.33	0.61
5:F:350:VAL:HG11	5:F:389:PHE:HA	1.81	0.61
6:D:789:LEU:HD13	6:D:806:LEU:HD13	1.82	0.61
1:B:735:GLU:HB2	1:B:738:ARG:HH21	1.65	0.61
2:C:1046:ARG:NH2	2:C:1186:GLN:O	2.33	0.61
5:F:12:ALA:O	5:F:36:LYS:NZ	2.34	0.61
1:B:827:SER:OG	1:B:828:MET:SD	2.58	0.61
6:D:567:ALA:O	6:D:571:HIS:ND1	2.34	0.61
6:D:508:SER:HA	6:D:511:ASN:HD22	1.66	0.60
6:D:666:GLN:O	6:D:669:THR:OG1	2.19	0.60
1:B:74:ASN:ND2	1:B:76:GLN:OE1	2.35	0.60
6:D:537:ALA:O	6:D:541:ASP:N	2.26	0.60
6:D:1336:THR:O	6:D:1339:THR:OG1	2.17	0.60
6:D:1557:SER:HA	6:D:1560:TRP:HD1	1.66	0.60
2:C:62:ILE:HG22	2:C:78:GLY:HA3	1.84	0.60
5:F:358:VAL:HG23	5:F:372:LEU:HD21	1.83	0.60
3:E:333:ARG:HG2	3:E:344:VAL:HG22	1.83	0.60
6:D:854:ILE:HD13	6:D:886:LYS:HZ3	1.67	0.60
6:D:1573:HIS:O	6:D:1601:ASN:ND2	2.34	0.60
3:E:1036:ILE:O	3:E:1040:THR:OG1	2.19	0.59
6:D:798:PHE:O	6:D:802:ALA:N	2.33	0.59
6:D:1002:ALA:O	6:D:1005:THR:OG1	2.19	0.59
1:B:874:MET:HE1	2:C:447:ASN:HB2	1.84	0.59
2:C:548:PHE:HB3	2:C:555:MET:HE1	1.84	0.59
6:D:447:TYR:OH	6:D:557:ASN:OD1	2.20	0.59
6:D:1225:GLU:OE2	6:D:1228:ARG:NH1	2.34	0.59
1:B:943:LYS:HE2	1:B:1001:LEU:HD22	1.83	0.59
1:B:946:TYR:HB3	1:B:994:ALA:HA	1.83	0.59
2:C:319:GLN:O	2:C:323:ASP:HA	2.03	0.59
6:D:327:VAL:O	6:D:331:ARG:N	2.33	0.59
1:B:1:MET:N	1:B:326:ASN:OD1	2.32	0.59
2:C:148:PRO:HD2	2:C:190:ARG:HH21	1.67	0.59
3:E:190:ARG:NH1	3:E:257:VAL:O	2.36	0.59
4:A:171:ARG:HH12	6:D:1323:VAL:HG23	1.68	0.59
2:C:627:GLU:HG3	2:C:630:ARG:HH12	1.68	0.59
6:D:867:SER:O	6:D:871:SER:N	2.35	0.59
6:D:1584:TRP:HE1	6:D:1589:GLU:HG3	1.67	0.59
1:B:42:LYS:HB3	1:B:57:SER:HB3	1.84	0.59
6:D:327:VAL:HG12	6:D:331:ARG:HE	1.68	0.59
6:D:1115:GLU:OE2	6:D:1119:GLN:NE2	2.35	0.59
2:C:1098:ILE:O	2:C:1200:ARG:NH1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:460:VAL:O	5:F:466:VAL:HA	2.01	0.59
6:D:1211:TYR:HE1	6:D:1248:ARG:HG3	1.68	0.58
6:D:1301:THR:OG1	6:D:1302:THR:N	2.32	0.58
1:B:91:VAL:HG13	1:B:102:GLU:HB3	1.85	0.58
3:E:829:PRO:HG2	3:E:854:ARG:HH11	1.68	0.58
1:B:83:SER:OG	1:B:84:ASP:N	2.35	0.58
3:E:365:THR:HA	3:E:378:PHE:O	2.03	0.58
1:B:633:ASP:OD2	1:B:636:ARG:NH2	2.37	0.58
6:D:333:LEU:O	6:D:338:ASP:N	2.35	0.58
6:D:1573:HIS:HD2	6:D:1601:ASN:HA	1.69	0.58
6:D:849:GLU:OE1	6:D:852:GLN:NE2	2.37	0.58
6:D:972:LEU:HA	6:D:975:GLN:HG2	1.85	0.58
2:C:406:LYS:HZ1	2:C:409:GLU:HB2	1.67	0.58
1:B:578:LEU:O	1:B:579:ARG:NH1	2.35	0.57
5:F:706:ILE:HD13	5:F:722:GLU:HG2	1.86	0.57
2:C:870:ALA:O	2:C:872:LYS:NZ	2.37	0.57
3:E:459:ASP:HB3	3:E:495:ILE:HG23	1.86	0.57
3:E:1077:SER:O	3:E:1081:THR:OG1	2.22	0.57
2:C:30:GLY:HA3	2:C:275:ARG:HH12	1.68	0.57
6:D:1034:MET:HA	6:D:1037:ILE:HD12	1.86	0.57
6:D:1509:PRO:HB2	6:D:1514:LEU:HD21	1.87	0.57
1:B:716:LEU:O	1:B:722:GLN:NE2	2.37	0.57
2:C:442:LYS:HE2	2:C:453:LEU:HD21	1.86	0.57
6:D:410:ALA:O	6:D:413:ARG:NH1	2.37	0.57
6:D:773:GLN:O	6:D:777:ALA:N	2.37	0.57
3:E:194:VAL:HG12	3:E:259:TYR:CZ	2.40	0.57
3:E:458:TRP:NE1	3:E:827:THR:OG1	2.36	0.57
1:B:1057:ARG:NH1	1:B:1060:GLN:OE1	2.35	0.57
2:C:179:ALA:HB3	2:C:201:SER:HB2	1.87	0.57
3:E:15:LEU:H	3:E:444:SER:HA	1.70	0.57
3:E:156:ARG:HE	3:E:183:GLN:HE21	1.53	0.57
5:F:635:GLY:HA2	5:F:651:LEU:HD12	1.85	0.57
6:D:1015:GLU:HA	6:D:1018:LEU:HD12	1.87	0.57
1:B:228:LEU:O	1:B:241:ASN:ND2	2.36	0.56
2:C:224:PHE:HB2	2:C:243:SER:H	1.70	0.56
2:C:1003:ARG:NH2	2:C:1030:ARG:O	2.38	0.56
2:C:1085:LEU:HA	2:C:1190:ALA:HB3	1.87	0.56
2:C:1223:MET:SD	2:C:1223:MET:N	2.78	0.56
5:F:794:GLN:O	5:F:797:GLU:HB3	2.05	0.56
2:C:235:GLY:O	2:C:252:LYS:NZ	2.39	0.56
5:F:656:ASN:ND2	5:F:665:GLU:OE1	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:754:SER:OG	5:F:755:SER:N	2.38	0.56
6:D:1479:MET:HG3	6:D:1544:PHE:HE1	1.70	0.56
2:C:82:THR:HA	2:C:97:GLN:HA	1.88	0.56
2:C:422:VAL:HG12	2:C:469:ARG:HH11	1.70	0.56
2:C:79:ALA:HA	2:C:101:ALA:HB1	1.87	0.56
5:F:20:VAL:HG11	5:F:59:ALA:HA	1.88	0.56
5:F:732:LEU:HD21	5:F:756:GLN:HB2	1.87	0.56
6:D:606:MET:SD	6:D:636:GLN:NE2	2.75	0.56
1:B:351:MET:HE1	1:B:353:TRP:HB2	1.86	0.56
2:C:857:ASP:O	3:E:996:ARG:NH1	2.39	0.56
5:F:573:VAL:HG22	5:F:585:THR:HG22	1.86	0.56
6:D:1161:LEU:HA	6:D:1164:LYS:HE2	1.87	0.56
2:C:37:CYS:SG	2:C:40:ARG:NH2	2.76	0.56
2:C:796:ASN:OD1	2:C:811:TYR:OH	2.23	0.56
5:F:163:LEU:HB3	5:F:176:ILE:HB	1.88	0.56
5:F:582:VAL:HG22	5:F:595:VAL:HG12	1.87	0.56
6:D:442:GLY:O	6:D:446:LEU:N	2.38	0.56
1:B:1186:GLN:HE21	1:B:1187:ARG:HE	1.54	0.56
6:D:334:MET:SD	6:D:335:GLN:NE2	2.79	0.56
1:B:190:LYS:NZ	1:B:237:GLU:O	2.38	0.56
2:C:520:THR:HA	2:C:534:ALA:HA	1.87	0.56
2:C:799:ARG:HE	2:C:800:LYS:HZ3	1.54	0.55
5:F:531:ARG:HH22	5:F:571:LYS:HD3	1.71	0.55
1:B:251:ILE:HB	1:B:260:LEU:HD11	1.87	0.55
2:C:349:GLN:OE1	2:C:376:ARG:NH2	2.39	0.55
2:C:416:VAL:HA	2:C:435:LEU:HA	1.87	0.55
3:E:14:GLN:N	3:E:34:VAL:O	2.34	0.55
3:E:650:GLN:OE1	3:E:653:ARG:NH2	2.40	0.55
6:D:1045:CYS:HB3	6:D:1083:ALA:HB2	1.87	0.55
1:B:606:GLU:OE2	1:B:651:ARG:NH2	2.40	0.55
1:B:819:TYR:HA	1:B:822:LEU:HB3	1.87	0.55
2:C:118:SER:OG	2:C:121:ASP:OD1	2.23	0.55
3:E:1204:ARG:HD2	3:E:1231:LEU:HD11	1.87	0.55
6:D:1455:GLN:OE1	6:D:1457:THR:N	2.39	0.55
3:E:1185:GLU:OE1	3:E:1197:TYR:OH	2.24	0.55
1:B:406:ARG:NH2	1:B:457:SER:OG	2.40	0.55
2:C:248:THR:HA	2:C:259:GLU:HA	1.87	0.55
2:C:1043:ARG:NH2	2:C:1048:ASN:OD1	2.40	0.55
3:E:1018:ALA:HA	3:E:1021:MET:HG2	1.88	0.55
6:D:800:ILE:O	6:D:804:SER:N	2.35	0.55
6:D:1475:LYS:NZ	6:D:1508:SER:OG	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:MET:HE1	1:B:15:VAL:HB	1.89	0.55
3:E:470:ASP:OD1	3:E:470:ASP:N	2.36	0.55
6:D:907:ASP:OD1	6:D:907:ASP:N	2.40	0.55
1:B:685:THR:O	1:B:690:ASP:N	2.37	0.55
6:D:1147:GLU:HA	6:D:1514:LEU:HD13	1.89	0.55
2:C:349:GLN:O	2:C:376:ARG:NE	2.39	0.54
6:D:957:THR:O	6:D:961:ARG:NH1	2.39	0.54
3:E:471:MET:HB3	3:E:483:LEU:HD11	1.90	0.54
6:D:445:GLN:HA	6:D:448:ARG:HB2	1.90	0.54
6:D:839:GLU:O	6:D:842:GLU:HB3	2.07	0.54
2:C:307:VAL:HG22	2:C:317:VAL:HG13	1.89	0.54
2:C:1013:ILE:HG22	5:F:730:LYS:HD3	1.89	0.54
3:E:547:ARG:HE	3:E:560:GLN:HA	1.71	0.54
1:B:529:MET:HG2	1:B:540:VAL:HG22	1.89	0.54
2:C:831:ARG:NH1	2:C:1277:GLU:OE2	2.40	0.54
2:C:1101:GLY:HA2	2:C:1200:ARG:HH22	1.73	0.54
3:E:260:ASP:O	3:E:264:ARG:N	2.40	0.54
3:E:711:GLU:OE1	3:E:870:ARG:NH1	2.41	0.54
3:E:886:ASP:O	5:F:798:TYR:OH	2.25	0.54
1:B:229:GLN:HG3	1:B:241:ASN:HB2	1.90	0.54
2:C:273:ARG:NH1	2:C:278:GLN:OE1	2.40	0.54
3:E:646:ARG:O	3:E:697:TRP:NE1	2.38	0.54
6:D:642:ASP:N	6:D:642:ASP:OD1	2.41	0.54
1:B:691:PHE:HB3	1:B:714:ARG:HD3	1.89	0.54
2:C:934:ARG:NH2	2:C:975:ALA:O	2.41	0.54
3:E:672:VAL:HG21	3:E:808:LEU:HD21	1.88	0.54
3:E:1020:ILE:HD12	3:E:1033:VAL:HG13	1.89	0.54
3:E:536:HIS:NE2	3:E:577:ASN:O	2.39	0.54
6:D:1084:ARG:HA	6:D:1087:LEU:HD23	1.89	0.54
2:C:160:GLY:HA2	2:C:181:VAL:HG23	1.89	0.54
2:C:510:ASP:OD1	2:C:510:ASP:N	2.40	0.54
6:D:408:ARG:NH1	6:D:554:VAL:O	2.41	0.54
1:B:165:LEU:HG	1:B:175:VAL:HG22	1.90	0.53
1:B:605:GLU:OE1	1:B:651:ARG:NH2	2.41	0.53
1:B:624:THR:HG23	1:B:643:VAL:HG23	1.89	0.53
1:B:753:ARG:NH2	1:B:758:ASP:OD2	2.40	0.53
2:C:1012:VAL:HG22	5:F:729:GLU:HA	1.89	0.53
3:E:375:LEU:HD11	3:E:439:LEU:HD11	1.90	0.53
5:F:163:LEU:HD23	5:F:176:ILE:HD12	1.89	0.53
1:B:824:GLN:NE2	1:B:827:SER:OG	2.42	0.53
2:C:28:PRO:O	2:C:275:ARG:NH2	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:412:MET:SD	2:C:412:MET:N	2.81	0.53
2:C:972:ALA:O	5:F:755:SER:OG	2.26	0.53
2:C:979:ASN:OD1	5:F:725:ARG:NH1	2.40	0.53
3:E:343:ASP:OD1	3:E:343:ASP:N	2.41	0.53
5:F:655:ASN:ND2	5:F:665:GLU:OE2	2.41	0.53
1:B:1005:GLN:NE2	1:B:1009:ASP:OD2	2.41	0.53
6:D:824:PHE:HB3	6:D:840:LEU:HD13	1.91	0.53
3:E:547:ARG:NH1	3:E:561:MET:O	2.42	0.53
5:F:161:PRO:HB2	5:F:178:LEU:HB2	1.90	0.53
5:F:611:VAL:HG21	5:F:619:LEU:HB2	1.89	0.53
5:F:677:ARG:NH1	5:F:701:ASP:OD2	2.41	0.53
3:E:674:ASP:O	3:E:678:ASP:CA	2.57	0.53
5:F:409:GLU:HB2	5:F:439:LEU:HD11	1.90	0.53
3:E:985:GLU:OE1	3:E:988:GLN:NE2	2.42	0.53
6:D:399:LEU:HA	6:D:402:PHE:HB2	1.89	0.53
6:D:451:ASP:O	6:D:455:THR:OG1	2.25	0.53
6:D:515:ARG:O	6:D:520:GLY:N	2.42	0.53
6:D:784:LYS:HZ1	6:D:788:LEU:HG	1.74	0.53
6:D:1475:LYS:HB3	6:D:1544:PHE:HZ	1.73	0.53
6:D:1540:LYS:O	6:D:1543:ARG:NH2	2.42	0.53
2:C:144:ALA:HB1	2:C:153:LEU:HD11	1.89	0.53
2:C:408:ARG:NH1	2:C:445:VAL:O	2.42	0.53
5:F:288:VAL:HG22	5:F:293:VAL:HG22	1.90	0.53
6:D:1352:PHE:HB3	6:D:1446:LEU:HD23	1.91	0.53
2:C:1016:VAL:HA	2:C:1019:MET:HE1	1.91	0.53
6:D:1533:ASP:HB3	6:D:1542:ALA:HB2	1.90	0.53
1:B:47:PRO:HA	1:B:50:GLN:HB2	1.91	0.53
6:D:1264:ARG:NE	6:D:1531:TYR:OH	2.38	0.53
1:B:310:VAL:HG13	1:B:321:ALA:HB3	1.90	0.53
1:B:493:SER:HB2	1:B:531:VAL:HG11	1.91	0.53
6:D:545:ARG:HB3	6:D:551:GLU:HB3	1.90	0.53
2:C:804:ILE:HD12	2:C:823:ILE:HD11	1.90	0.52
3:E:1157:ALA:HA	3:E:1160:SER:HB3	1.89	0.52
3:E:1208:ARG:HA	3:E:1211:TRP:CD1	2.44	0.52
2:C:34:VAL:HG22	2:C:43:VAL:HG22	1.90	0.52
3:E:572:ILE:HB	3:E:583:VAL:HB	1.91	0.52
3:E:674:ASP:O	3:E:678:ASP:HA	2.08	0.52
6:D:974:ASP:OD1	6:D:974:ASP:N	2.35	0.52
6:D:977:TRP:NE1	6:D:997:ASP:OD2	2.42	0.52
6:D:1574:LYS:O	6:D:1577:SER:OG	2.27	0.52
1:B:72:THR:HG22	1:B:81:THR:HB	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:906:ARG:NH2	1:B:908:THR:OG1	2.42	0.52
2:C:994:ASN:ND2	2:C:1025:GLU:OE2	2.43	0.52
2:C:1218:ARG:NH2	2:C:1220:TYR:OH	2.38	0.52
6:D:954:ALA:N	6:D:957:THR:OG1	2.43	0.52
6:D:1342:PRO:HA	6:D:1345:LEU:HD13	1.92	0.52
2:C:309:ARG:HD2	2:C:312:MET:HA	1.92	0.52
2:C:693:ASP:N	2:C:693:ASP:OD1	2.41	0.52
3:E:657:MET:HG2	3:E:670:ILE:HD11	1.90	0.52
5:F:387:PRO:HA	5:F:401:VAL:HG13	1.90	0.52
5:F:350:VAL:HG12	5:F:390:ILE:HG12	1.91	0.52
6:D:589:GLU:O	6:D:593:ARG:N	2.42	0.52
1:B:372:ASN:OD1	1:B:373:ALA:N	2.41	0.52
3:E:65:PRO:HA	3:E:81:TRP:HA	1.91	0.52
3:E:466:GLN:NE2	3:E:468:SER:O	2.42	0.52
3:E:481:GLN:NE2	3:E:848:TYR:O	2.43	0.52
3:E:595:SER:OG	3:E:598:ASP:OD1	2.27	0.52
6:D:789:LEU:HD22	6:D:806:LEU:HB2	1.92	0.52
6:D:1567:TYR:HB2	6:D:1576:ALA:HB2	1.91	0.52
6:D:1462:VAL:HG22	6:D:1465:ARG:HH21	1.75	0.52
5:F:848:ILE:HG21	5:F:875:LEU:HB2	1.92	0.52
6:D:1613:ASP:OD1	6:D:1613:ASP:N	2.42	0.52
3:E:1185:GLU:OE2	3:E:1208:ARG:NH1	2.42	0.52
6:D:1148:GLN:N	6:D:1148:GLN:OE1	2.42	0.52
1:B:370:TYR:OH	1:B:372:ASN:ND2	2.36	0.52
2:C:608:ARG:HG2	2:C:623:LEU:HD23	1.91	0.52
6:D:304:LEU:HA	6:D:307:ALA:HB3	1.92	0.52
6:D:962:ILE:HD12	6:D:962:ILE:H	1.75	0.52
6:D:1534:THR:OG1	6:D:1535:GLN:NE2	2.42	0.52
1:B:23:ASN:HB2	1:B:73:TRP:CD2	2.44	0.51
2:C:505:ASN:ND2	2:C:543:LYS:O	2.43	0.51
3:E:674:ASP:O	3:E:678:ASP:N	2.43	0.51
6:D:745:ASP:N	6:D:745:ASP:OD1	2.38	0.51
6:D:1010:GLN:HG2	6:D:1034:MET:HB3	1.92	0.51
1:B:212:ARG:NH1	1:B:345:LYS:O	2.44	0.51
1:B:547:THR:HG21	1:B:575:VAL:HB	1.92	0.51
6:D:883:ASP:HB2	6:D:886:LYS:HG2	1.92	0.51
1:B:1230:ARG:NE	1:B:1231:ASN:OD1	2.43	0.51
3:E:813:PHE:O	3:E:856:ARG:NH1	2.44	0.51
3:E:869:VAL:HG13	3:E:895:ILE:HG23	1.93	0.51
5:F:202:VAL:HB	5:F:209:LEU:HB3	1.92	0.51
5:F:224:ASN:HB3	5:F:227:LEU:HG	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:439:CYS:SG	6:D:440:GLY:N	2.83	0.51
3:E:71:HIS:HB2	3:E:76:LEU:HB3	1.92	0.51
6:D:515:ARG:HG2	6:D:519:ARG:HD2	1.92	0.51
5:F:404:GLN:HB3	5:F:443:GLU:HG3	1.92	0.51
1:B:264:ALA:HB3	1:B:277:VAL:HG13	1.92	0.51
6:D:753:LEU:HD13	6:D:773:GLN:HG2	1.92	0.51
1:B:106:ASN:O	1:B:108:ASN:ND2	2.43	0.51
2:C:272:GLN:NE2	2:C:273:ARG:O	2.36	0.51
3:E:943:ASP:O	3:E:947:GLN:NE2	2.44	0.51
3:E:1228:ASP:HB3	3:E:1231:LEU:HD23	1.92	0.51
5:F:595:VAL:HG11	5:F:673:LEU:HA	1.91	0.51
1:B:107:ARG:NH1	1:B:109:SER:OG	2.44	0.50
1:B:340:PHE:HE1	1:B:351:MET:HB2	1.76	0.50
1:B:460:ARG:HG2	1:B:474:PRO:HB3	1.93	0.50
2:C:507:ASP:HB2	2:C:544:ALA:HB2	1.92	0.50
2:C:1260:ARG:O	2:C:1267:ARG:NH2	2.45	0.50
3:E:155:GLN:O	3:E:183:GLN:NE2	2.44	0.50
3:E:507:GLN:HB3	3:E:527:LEU:HD23	1.92	0.50
5:F:745:LYS:NZ	5:F:749:ASN:OD1	2.44	0.50
6:D:1217:GLU:HB3	6:D:1222:ASN:HB3	1.92	0.50
1:B:106:ASN:ND2	1:B:108:ASN:OD1	2.45	0.50
1:B:638:ARG:NH1	1:B:640:ASP:OD2	2.44	0.50
1:B:806:TYR:HA	1:B:809:LEU:HD12	1.93	0.50
1:B:842:MET:O	1:B:845:THR:OG1	2.25	0.50
2:C:38:GLY:HA2	2:C:61:THR:HG23	1.94	0.50
2:C:923:ALA:HB2	5:F:827:VAL:HG11	1.91	0.50
6:D:498:GLN:NE2	6:D:499:PRO:O	2.44	0.50
6:D:923:GLU:HA	6:D:926:VAL:HG22	1.93	0.50
6:D:506:GLU:HA	6:D:509:MET:HG2	1.93	0.50
6:D:1123:THR:HA	6:D:1126:ARG:NE	2.26	0.50
1:B:168:THR:HG1	1:B:172:GLU:H	1.60	0.50
1:B:366:ARG:NH1	1:B:384:PRO:O	2.44	0.50
2:C:617:THR:HA	2:C:620:VAL:HG12	1.94	0.50
2:C:1218:ARG:NH2	2:C:1220:TYR:HH	2.09	0.50
3:E:695:VAL:HB	3:E:715:LEU:HD11	1.93	0.50
6:D:633:LEU:HD11	6:D:643:ALA:HB3	1.94	0.50
6:D:979:VAL:HG11	6:D:1072:VAL:HG22	1.92	0.50
1:B:699:ILE:HD11	2:C:714:LEU:HA	1.92	0.50
2:C:764:ILE:HD12	2:C:790:LEU:HD23	1.92	0.50
3:E:934:ARG:NH1	5:F:766:ASP:OD2	2.42	0.50
5:F:677:ARG:O	5:F:680:SER:OG	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1230:ARG:NH1	4:A:190:ASP:OD1	2.44	0.50
6:D:311:LEU:HD13	6:D:329:LYS:HA	1.93	0.50
6:D:590:LYS:O	6:D:590:LYS:NZ	2.40	0.50
6:D:969:TYR:O	6:D:973:ARG:N	2.45	0.50
3:E:149:LEU:HB3	3:E:161:TRP:HB2	1.93	0.50
3:E:645:ALA:HA	3:E:655:ALA:O	2.11	0.50
3:E:698:ASN:ND2	3:E:711:GLU:O	2.43	0.50
3:E:1017:ASP:N	3:E:1017:ASP:OD1	2.44	0.50
3:E:1205:SER:OG	3:E:1208:ARG:NH2	2.44	0.50
5:F:660:ARG:NH1	5:F:681:ASN:OD1	2.44	0.50
6:D:857:TYR:HB3	6:D:874:VAL:HG22	1.94	0.50
6:D:1140:LEU:O	6:D:1144:LEU:N	2.44	0.50
1:B:659:ASP:OD1	1:B:659:ASP:N	2.41	0.50
6:D:507:LEU:O	6:D:511:ASN:ND2	2.45	0.50
6:D:1460:ARG:HH12	6:D:1538:ARG:HH22	1.60	0.50
6:D:1539:LEU:HD12	6:D:1540:LYS:HD3	1.93	0.50
1:B:189:ILE:HD13	1:B:231:MET:HE1	1.94	0.49
2:C:118:SER:OG	2:C:121:ASP:O	2.26	0.49
2:C:461:LYS:HE2	2:C:475:ILE:HD11	1.93	0.49
2:C:677:ASP:OD1	2:C:677:ASP:N	2.44	0.49
2:C:1281:ALA:HA	2:C:1284:LYS:HG2	1.92	0.49
3:E:417:MET:HA	3:E:794:ARG:HE	1.77	0.49
2:C:1:MET:HE1	2:C:295:ILE:HA	1.94	0.49
2:C:163:MET:HA	2:C:174:ILE:HG12	1.93	0.49
3:E:1190:ASP:N	3:E:1190:ASP:OD1	2.41	0.49
3:E:422:VAL:HG13	3:E:424:LYS:H	1.78	0.49
6:D:1333:ALA:O	6:D:1337:MET:HG2	2.12	0.49
6:D:1624:THR:O	6:D:1624:THR:OG1	2.28	0.49
3:E:885:MET:HE1	3:E:908:CYS:HA	1.95	0.49
5:F:599:HIS:O	5:F:599:HIS:ND1	2.41	0.49
6:D:1081:THR:HB	6:D:1084:ARG:HH21	1.76	0.49
1:B:747:ASP:OD1	1:B:747:ASP:N	2.43	0.49
3:E:260:ASP:O	3:E:264:ARG:CA	2.60	0.49
3:E:641:SER:OG	3:E:659:THR:OG1	2.31	0.49
5:F:769:GLN:HB3	5:F:772:ARG:HG2	1.95	0.49
3:E:1047:ARG:HE	3:E:1093:TRP:HZ2	1.60	0.49
1:B:401:SER:HB2	2:C:561:PRO:HA	1.93	0.49
1:B:1026:ASP:HB2	1:B:1031:PRO:HG3	1.95	0.49
2:C:66:ASP:OD2	2:C:107:HIS:ND1	2.43	0.49
2:C:850:PRO:HA	2:C:853:THR:HG22	1.95	0.49
3:E:1217:GLY:O	3:E:1221:ASN:ND2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:786:PRO:O	5:F:789:SER:HB2	2.12	0.49
6:D:851:GLU:HA	6:D:854:ILE:HD12	1.95	0.49
1:B:26:GLN:OE1	1:B:28:TRP:NE1	2.40	0.49
2:C:1046:ARG:HD2	2:C:1066:HIS:HB2	1.94	0.49
5:F:659:LEU:HD13	5:F:661:THR:HG22	1.93	0.49
6:D:1070:LEU:O	6:D:1073:GLN:NE2	2.38	0.49
3:E:331:ARG:HE	3:E:344:VAL:HG11	1.77	0.49
3:E:493:VAL:HG22	3:E:502:LEU:HD22	1.95	0.49
5:F:770:TRP:H	5:F:770:TRP:CD1	2.31	0.49
1:B:716:LEU:HD21	1:B:721:LYS:HB3	1.93	0.49
1:B:943:LYS:HZ3	1:B:944:LYS:HE3	1.77	0.49
2:C:1245:GLU:OE1	3:E:1205:SER:OG	2.30	0.49
3:E:1202:ALA:HB1	3:E:1205:SER:HB2	1.95	0.49
5:F:116:LYS:HG2	5:F:140:ARG:HG3	1.94	0.49
6:D:1158:PHE:O	6:D:1161:LEU:HB3	2.13	0.49
1:B:1173:PRO:HA	1:B:1180:PHE:HA	1.95	0.48
2:C:438:GLY:O	2:C:456:GLY:N	2.46	0.48
1:B:649:LEU:HD21	1:B:677:LEU:HD11	1.95	0.48
1:B:863:ARG:NH2	1:B:889:ASP:OD2	2.46	0.48
1:B:917:ALA:HB1	1:B:919:LYS:HE2	1.94	0.48
6:D:1194:ARG:O	6:D:1198:ALA:N	2.46	0.48
1:B:420:SER:HB2	1:B:436:ARG:HH21	1.78	0.48
5:F:770:TRP:HE3	5:F:788:ILE:HG22	1.77	0.48
6:D:327:VAL:HB	6:D:331:ARG:HH21	1.79	0.48
1:B:1:MET:HB3	1:B:325:PRO:HA	1.93	0.48
2:C:132:VAL:HB	2:C:134:LYS:HE3	1.94	0.48
3:E:140:SER:HA	3:E:150:VAL:O	2.12	0.48
5:F:837:GLU:OE2	5:F:840:ARG:NH1	2.46	0.48
6:D:550:MET:HE3	6:D:550:MET:HB3	1.78	0.48
1:B:493:SER:OG	1:B:494:GLU:N	2.46	0.48
1:B:577:ASN:OD1	1:B:578:LEU:N	2.46	0.48
1:B:1049:GLY:HA3	1:B:1166:ASP:HB2	1.95	0.48
3:E:495:ILE:HB	3:E:500:ILE:HD12	1.96	0.48
4:A:171:ARG:NE	6:D:1319:LEU:O	2.46	0.48
5:F:903:ILE:HD13	5:F:924:ILE:HG23	1.94	0.48
6:D:509:MET:SD	6:D:509:MET:N	2.86	0.48
2:C:817:HIS:HA	2:C:820:LEU:HD12	1.95	0.48
3:E:6:VAL:HG22	3:E:449:LEU:HG	1.95	0.48
3:E:855:LEU:HB2	3:E:858:PHE:HB2	1.94	0.48
6:D:389:ARG:HH22	6:D:422:GLN:HB3	1.78	0.48
1:B:1002:MET:HA	1:B:1005:GLN:HG3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:969:GLY:O	2:C:1059:ASP:N	2.45	0.48
6:D:315:PHE:HB3	6:D:325:PRO:HG2	1.94	0.48
6:D:456:GLU:HA	6:D:459:ARG:HD2	1.96	0.48
6:D:1122:THR:O	6:D:1126:ARG:HG3	2.13	0.48
2:C:80:ASP:OD2	2:C:82:THR:OG1	2.31	0.48
3:E:669:ARG:HA	3:E:684:ASP:HA	1.96	0.48
6:D:798:PHE:O	6:D:801:ALA:HB3	2.14	0.48
1:B:354:ASN:O	1:B:358:ASN:N	2.47	0.48
2:C:926:ILE:HG13	2:C:1213:LEU:HD13	1.94	0.48
2:C:1061:CYS:HB3	2:C:1066:HIS:H	1.79	0.48
6:D:1155:ARG:NH2	6:D:1159:GLU:OE2	2.46	0.48
1:B:934:ALA:HB1	1:B:941:LYS:HE3	1.95	0.48
2:C:202:TRP:NE1	2:C:226:PRO:O	2.42	0.48
3:E:1223:ALA:O	3:E:1226:SER:OG	2.26	0.48
5:F:469:SER:HB3	5:F:480:PRO:HB3	1.96	0.48
6:D:766:ILE:O	6:D:769:VAL:HB	2.13	0.48
2:C:36:SER:HB2	2:C:62:ILE:HG13	1.94	0.47
2:C:251:THR:OG1	2:C:253:ASP:OD1	2.30	0.47
2:C:385:THR:OG1	2:C:388:ALA:O	2.31	0.47
2:C:433:VAL:O	2:C:440:VAL:HA	2.14	0.47
3:E:547:ARG:CZ	3:E:561:MET:H	2.27	0.47
3:E:604:PRO:O	3:E:606:ARG:NE	2.46	0.47
3:E:658:SER:OG	3:E:667:ASP:OD2	2.27	0.47
3:E:667:ASP:OD2	3:E:669:ARG:NH1	2.46	0.47
5:F:700:LEU:HD21	5:F:734:LEU:HD23	1.95	0.47
5:F:706:ILE:HG23	5:F:718:VAL:HG13	1.96	0.47
1:B:717:ASP:OD1	1:B:717:ASP:N	2.47	0.47
3:E:539:GLY:HA3	3:E:551:GLU:O	2.14	0.47
3:E:670:ILE:HG12	3:E:695:VAL:HG11	1.95	0.47
5:F:629:PRO:HB3	5:F:637:VAL:HG11	1.95	0.47
1:B:217:ALA:HB1	1:B:230:LEU:HB3	1.96	0.47
2:C:569:TYR:HD1	2:C:574:ASP:HB3	1.79	0.47
3:E:18:GLN:HG2	3:E:19:LEU:HG	1.96	0.47
5:F:614:SER:OG	5:F:617:ASP:OD1	2.32	0.47
6:D:1257:THR:OG1	6:D:1258:THR:N	2.44	0.47
6:D:1264:ARG:NH2	6:D:1535:GLN:OE1	2.46	0.47
1:B:620:LEU:HD12	1:B:676:LYS:HB3	1.97	0.47
1:B:849:ALA:HB2	1:B:872:VAL:HG11	1.95	0.47
6:D:525:THR:O	6:D:529:ARG:HG2	2.15	0.47
6:D:994:ASN:HB2	6:D:1000:LEU:HD22	1.96	0.47
6:D:1181:HIS:HA	6:D:1553:ASN:OD1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1257:THR:OG1	6:D:1259:GLN:OE1	2.25	0.47
1:B:116:ALA:HB1	1:B:157:TRP:HD1	1.79	0.47
6:D:767:GLY:O	6:D:770:ILE:HG12	2.15	0.47
1:B:110:SER:HG	1:B:128:TYR:HB3	1.78	0.47
2:C:249:LEU:HD22	2:C:260:LEU:HD11	1.96	0.47
6:D:1437:VAL:HG22	6:D:1465:ARG:HH11	1.78	0.47
6:D:1633:MET:SD	6:D:1633:MET:N	2.87	0.47
2:C:439:GLN:HB3	2:C:441:MET:HE2	1.96	0.47
5:F:331:LEU:HD21	5:F:345:LEU:HD22	1.97	0.47
6:D:1000:LEU:HA	6:D:1003:LEU:HD23	1.96	0.47
6:D:1011:ARG:HA	6:D:1014:LEU:HD12	1.95	0.47
6:D:1526:MET:HE2	6:D:1526:MET:HB3	1.60	0.47
1:B:191:CYS:SG	1:B:229:GLN:NE2	2.88	0.47
1:B:864:MET:HE2	1:B:864:MET:HB2	1.77	0.47
2:C:774:GLU:O	2:C:778:LYS:NZ	2.44	0.47
3:E:650:GLN:HE21	3:E:712:TYR:HB2	1.80	0.47
5:F:388:ALA:N	5:F:400:GLY:O	2.47	0.47
2:C:76:SER:OG	2:C:86:TRP:NE1	2.34	0.47
3:E:276:GLU:OE1	3:E:278:TYR:OH	2.23	0.47
3:E:962:VAL:HG12	3:E:966:ARG:HG3	1.97	0.47
6:D:802:ALA:O	6:D:805:GLN:HG3	2.15	0.47
2:C:247:VAL:O	2:C:260:LEU:N	2.44	0.47
1:B:26:GLN:HB2	1:B:28:TRP:CD1	2.49	0.46
1:B:1035:TYR:HD1	1:B:1038:ILE:HD12	1.80	0.46
2:C:77:GLY:HA3	2:C:102:ILE:HD11	1.97	0.46
3:E:693:ASN:HB2	3:E:720:TYR:HE2	1.80	0.46
3:E:897:ASN:HD21	3:E:899:ALA:HB3	1.80	0.46
3:E:1107:LEU:O	3:E:1111:ASN:ND2	2.33	0.46
6:D:374:HIS:O	6:D:377:ALA:N	2.37	0.46
6:D:1250:ILE:HD11	6:D:1317:LEU:HB3	1.96	0.46
1:B:469:ARG:HA	1:B:515:GLN:HG2	1.97	0.46
2:C:718:ASP:OD1	2:C:718:ASP:N	2.48	0.46
3:E:28:LEU:HD23	3:E:41:ILE:HD11	1.97	0.46
6:D:671:ASP:OD1	6:D:672:PHE:N	2.48	0.46
6:D:1123:THR:O	6:D:1127:MET:HG3	2.15	0.46
1:B:899:LYS:O	1:B:899:LYS:NZ	2.38	0.46
1:B:1002:MET:HE3	1:B:1002:MET:HB3	1.82	0.46
2:C:438:GLY:HA2	2:C:460:VAL:HG23	1.97	0.46
2:C:895:ARG:NH2	2:C:1255:PRO:O	2.42	0.46
6:D:529:ARG:O	6:D:533:GLN:N	2.48	0.46
6:D:664:LEU:O	6:D:680:TYR:OH	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:ALA:HB3	2:C:115:ALA:HB3	1.96	0.46
2:C:246:LYS:HG2	2:C:262:SER:HA	1.98	0.46
2:C:441:MET:SD	2:C:452:LEU:HA	2.55	0.46
2:C:505:ASN:OD1	2:C:508:VAL:N	2.36	0.46
5:F:387:PRO:HB3	5:F:399:ALA:HB1	1.97	0.46
6:D:312:ASP:OD1	6:D:329:LYS:NZ	2.45	0.46
6:D:374:HIS:O	6:D:376:ALA:N	2.48	0.46
1:B:869:CYS:HA	1:B:872:VAL:HG12	1.96	0.46
1:B:882:ALA:HA	1:B:887:LEU:HD12	1.97	0.46
2:C:573:ARG:HB3	2:C:603:ARG:HH12	1.81	0.46
2:C:1083:PHE:HD2	2:C:1190:ALA:HB2	1.80	0.46
1:B:794:SER:OG	1:B:795:LYS:NZ	2.49	0.46
2:C:125:TRP:HZ3	2:C:130:PRO:HA	1.81	0.46
5:F:160:ASP:OD1	5:F:160:ASP:N	2.38	0.46
5:F:533:PHE:CD1	5:F:573:VAL:HB	2.50	0.46
6:D:645:LEU:HD21	6:D:664:LEU:HA	1.97	0.46
6:D:1094:ASP:OD1	6:D:1096:SER:OG	2.34	0.46
1:B:106:ASN:N	1:B:106:ASN:OD1	2.48	0.46
1:B:371:MET:HE3	1:B:371:MET:HB2	1.75	0.46
1:B:997:TYR:CZ	1:B:1000:LEU:HD23	2.51	0.46
3:E:1:MET:O	3:E:693:ASN:ND2	2.44	0.46
3:E:470:ASP:HA	3:E:490:VAL:HG23	1.97	0.46
5:F:788:ILE:H	5:F:788:ILE:HG13	1.52	0.46
6:D:770:ILE:O	6:D:773:GLN:HB2	2.15	0.46
6:D:1462:VAL:O	6:D:1465:ARG:NH2	2.49	0.46
1:B:1231:ASN:HB3	1:B:1236:HIS:HA	1.98	0.46
2:C:1009:LEU:HD11	2:C:1014:LEU:HD11	1.98	0.46
2:C:1241:ALA:HB1	3:E:1204:ARG:HD3	1.97	0.46
5:F:570:GLN:HA	5:F:587:ASP:HB3	1.98	0.46
1:B:466:ASP:OD2	1:B:479:ARG:NH1	2.47	0.46
1:B:768:GLU:N	1:B:768:GLU:OE1	2.49	0.46
2:C:190:ARG:NH1	2:C:195:ASP:OD1	2.49	0.46
3:E:254:ILE:HD11	3:E:268:THR:HB	1.98	0.46
3:E:832:LEU:HD23	3:E:850:ILE:HD11	1.98	0.46
5:F:535:ASN:OD1	5:F:539:THR:N	2.45	0.46
6:D:321:CYS:O	6:D:323:ILE:N	2.43	0.46
6:D:997:ASP:OD1	6:D:1000:LEU:N	2.46	0.46
2:C:1078:LEU:HD13	2:C:1229:VAL:HG13	1.98	0.46
6:D:452:LYS:HE2	6:D:481:GLN:HG2	1.96	0.46
6:D:1479:MET:HE1	6:D:1507:LEU:HA	1.98	0.46
1:B:614:LEU:HD12	1:B:624:THR:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:HIS:O	1:B:688:GLN:HG3	2.16	0.45
1:B:1205:ILE:HG21	1:B:1211:ALA:HB2	1.98	0.45
5:F:449:THR:OG1	5:F:461:VAL:O	2.31	0.45
5:F:857:MET:HE1	5:F:888:LEU:HD11	1.98	0.45
1:B:808:LYS:O	1:B:812:ILE:HG12	2.16	0.45
1:B:1004:GLN:NE2	4:A:182:CYS:O	2.49	0.45
2:C:837:LEU:HG	2:C:847:VAL:HG21	1.98	0.45
1:B:483:THR:OG1	1:B:485:ASP:OD1	2.33	0.45
2:C:43:VAL:HB	2:C:53:HIS:HB2	1.97	0.45
2:C:231:TYR:HB3	2:C:235:GLY:HA2	1.97	0.45
6:D:753:LEU:HD22	6:D:773:GLN:HG2	1.98	0.45
1:B:114:ASP:HB3	1:B:155:VAL:HG12	1.97	0.45
2:C:967:LEU:HB3	2:C:985:ILE:HD13	1.97	0.45
3:E:33:TRP:HE1	3:E:40:LEU:HB2	1.82	0.45
3:E:1229:GLU:O	3:E:1233:LEU:HB2	2.17	0.45
6:D:616:TRP:O	6:D:619:THR:OG1	2.23	0.45
6:D:1634:ASP:OD1	6:D:1634:ASP:N	2.50	0.45
3:E:879:TYR:CZ	3:E:887:GLU:HB3	2.51	0.45
5:F:100:CYS:SG	5:F:101:PHE:N	2.90	0.45
5:F:473:ASP:OD1	5:F:473:ASP:N	2.47	0.45
6:D:967:LEU:O	6:D:971:VAL:HG13	2.17	0.45
1:B:664:GLU:O	1:B:667:GLU:HG3	2.16	0.45
1:B:835:LEU:HD12	1:B:835:LEU:H	1.82	0.45
2:C:149:ASN:OD1	2:C:190:ARG:NH2	2.49	0.45
2:C:401:ASP:OD1	2:C:405:ASN:N	2.50	0.45
3:E:4:PHE:CD1	3:E:449:LEU:HB3	2.52	0.45
3:E:458:TRP:HE1	3:E:827:THR:HG1	1.63	0.45
3:E:1215:GLN:OE1	3:E:1218:VAL:N	2.43	0.45
1:B:18:THR:OG1	1:B:68:VAL:O	2.32	0.45
1:B:105:ASN:OD1	1:B:106:ASN:N	2.50	0.45
1:B:940:LEU:O	1:B:943:LYS:NZ	2.47	0.45
2:C:508:VAL:HB	2:C:511:ASN:ND2	2.31	0.45
2:C:696:ARG:HA	2:C:699:MET:HE2	1.98	0.45
3:E:456:ARG:HD2	3:E:824:VAL:HG22	1.99	0.45
3:E:551:GLU:HB3	3:E:555:LEU:HA	1.98	0.45
3:E:844:ASN:HD22	3:E:847:ASP:HB2	1.82	0.45
3:E:863:SER:HB3	3:E:866:ASP:HB2	1.98	0.45
6:D:755:GLU:HG2	6:D:759:LYS:HE2	1.97	0.45
6:D:1308:HIS:O	6:D:1312:ARG:HG2	2.17	0.45
6:D:1473:THR:HA	6:D:1476:MET:HE1	1.98	0.45
6:D:1567:TYR:HD1	6:D:1572:LYS:HZ1	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1172:LEU:HD12	2:C:1173:GLN:HG3	1.99	0.45
6:D:516:TRP:HA	6:D:520:GLY:HA3	1.97	0.45
6:D:527:VAL:O	6:D:531:LEU:N	2.41	0.45
3:E:815:PRO:HD2	3:E:856:ARG:HH22	1.82	0.45
5:F:36:LYS:HD2	5:F:38:ARG:HE	1.81	0.45
6:D:1085:GLU:HA	6:D:1088:ARG:NH2	2.32	0.45
2:C:481:LEU:HD12	2:C:499:VAL:HG11	1.98	0.45
3:E:933:LEU:HD21	3:E:951:LEU:HA	1.98	0.45
4:A:167:LEU:HA	4:A:170:MET:HG2	1.99	0.45
5:F:721:LEU:HD23	5:F:724:ILE:HD11	1.98	0.45
6:D:1106:GLN:HB3	6:D:1110:ARG:NH2	2.32	0.45
6:D:1135:ALA:O	6:D:1139:ILE:HG22	2.16	0.45
6:D:1541:ASP:HA	6:D:1544:PHE:HB3	1.98	0.45
1:B:578:LEU:HG	1:B:590:VAL:HG22	1.98	0.44
3:E:501:ALA:HA	3:E:510:PHE:HA	1.99	0.44
3:E:1043:MET:HE1	3:E:1100:ARG:HH12	1.82	0.44
6:D:1038:CYS:SG	6:D:1090:ALA:HA	2.57	0.44
1:B:7:LYS:HB3	1:B:320:PHE:HB2	1.98	0.44
1:B:146:ARG:NH2	1:B:180:SER:O	2.50	0.44
1:B:378:CYS:SG	1:B:379:VAL:N	2.89	0.44
1:B:1179:SER:O	1:B:1181:ASN:ND2	2.50	0.44
3:E:536:HIS:HB2	3:E:575:ILE:HD13	1.99	0.44
5:F:36:LYS:HG3	5:F:38:ARG:HG2	1.97	0.44
6:D:812:THR:O	6:D:815:HIS:NE2	2.50	0.44
6:D:1109:TYR:CG	6:D:1140:LEU:HD11	2.53	0.44
6:D:1309:ASP:HA	6:D:1312:ARG:HG2	1.98	0.44
6:D:1531:TYR:O	6:D:1534:THR:OG1	2.28	0.44
1:B:897:TYR:OH	1:B:909:GLU:OE2	2.29	0.44
2:C:177:ARG:NH1	2:C:209:TYR:OH	2.49	0.44
3:E:1213:MET:HB2	3:E:1215:GLN:HB2	1.99	0.44
5:F:633:PHE:O	5:F:636:THR:OG1	2.32	0.44
6:D:587:VAL:HA	6:D:590:LYS:HB3	1.99	0.44
6:D:769:VAL:O	6:D:772:ALA:HB3	2.18	0.44
6:D:1239:ASN:OD1	6:D:1242:CYS:N	2.50	0.44
2:C:379:CYS:HA	2:C:393:ASN:HB2	2.00	0.44
3:E:568:GLY:HA3	3:E:586:LYS:NZ	2.31	0.44
3:E:1076:GLN:HA	3:E:1079:PHE:HD2	1.83	0.44
2:C:884:LEU:HB3	2:C:900:TYR:CE2	2.53	0.44
5:F:771:GLU:H	5:F:771:GLU:CD	2.25	0.44
6:D:1311:ILE:HD13	6:D:1339:THR:HA	1.99	0.44
1:B:408:ILE:HG22	1:B:410:MET:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:LYS:NZ	1:B:701:CYS:O	2.51	0.44
1:B:710:VAL:HA	1:B:713:VAL:HG22	2.00	0.44
1:B:1213:GLN:NE2	1:B:1214:CYS:O	2.42	0.44
2:C:319:GLN:O	2:C:323:ASP:CA	2.65	0.44
2:C:472:LEU:HB2	2:C:486:LEU:HD11	1.99	0.44
2:C:872:LYS:HA	2:C:872:LYS:HD3	1.90	0.44
3:E:184:SER:OG	3:E:186:GLU:O	2.35	0.44
3:E:258:LEU:HD23	3:E:258:LEU:HA	1.87	0.44
3:E:1020:ILE:HD11	3:E:1036:ILE:HB	1.99	0.44
6:D:878:LEU:HD21	6:D:890:TYR:CD2	2.53	0.44
6:D:1059:MET:SD	6:D:1059:MET:N	2.91	0.44
2:C:380:SER:N	2:C:392:SER:O	2.49	0.44
2:C:675:ALA:N	2:C:678:SER:HG	2.16	0.44
3:E:254:ILE:HD12	3:E:254:ILE:HA	1.78	0.44
6:D:334:MET:HE2	6:D:334:MET:HB2	1.90	0.44
2:C:419:MET:HE1	2:C:431:LEU:HB3	1.99	0.44
3:E:246:PRO:O	3:E:285:LYS:NZ	2.50	0.44
6:D:354:LYS:HE3	6:D:383:ARG:HD2	2.00	0.44
6:D:413:ARG:H	6:D:413:ARG:HD2	1.83	0.44
6:D:962:ILE:HA	6:D:965:TYR:HD2	1.83	0.44
1:B:502:GLU:HB2	1:B:525:ARG:HH21	1.82	0.43
1:B:720:LYS:HB3	1:B:720:LYS:HE3	1.73	0.43
2:C:277:LYS:HA	2:C:277:LYS:HD3	1.88	0.43
2:C:531:TYR:HB2	2:C:564:HIS:CD2	2.53	0.43
3:E:248:VAL:HG12	3:E:286:GLY:HA3	1.98	0.43
5:F:614:SER:OG	5:F:617:ASP:O	2.34	0.43
5:F:687:GLN:OE1	5:F:687:GLN:N	2.44	0.43
6:D:840:LEU:O	6:D:843:ALA:HB3	2.18	0.43
1:B:114:ASP:OD1	1:B:115:PHE:N	2.50	0.43
1:B:600:ASN:OD1	1:B:601:HIS:ND1	2.43	0.43
3:E:546:ASN:ND2	3:E:568:GLY:O	2.51	0.43
6:D:870:LEU:O	6:D:874:VAL:HG23	2.18	0.43
1:B:443:ASP:OD1	1:B:446:ASP:N	2.43	0.43
2:C:21:VAL:HG23	2:C:286:GLY:HA2	2.00	0.43
2:C:390:ILE:HG13	2:C:399:MET:HG3	2.00	0.43
6:D:356:ASN:HD21	6:D:358:GLU:HB3	1.83	0.43
6:D:606:MET:HA	6:D:609:GLN:HB3	2.00	0.43
6:D:1594:VAL:HA	6:D:1597:LYS:HB2	2.00	0.43
1:B:251:ILE:HA	1:B:261:ALA:O	2.19	0.43
1:B:475:THR:OG1	1:B:476:MET:N	2.51	0.43
2:C:1:MET:SD	2:C:296:SER:OG	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:622:LEU:O	2:C:625:SER:OG	2.36	0.43
3:E:260:ASP:O	3:E:264:ARG:HA	2.17	0.43
6:D:475:VAL:HG13	6:D:487:ALA:HA	2.00	0.43
1:B:685:THR:HB	1:B:690:ASP:HB3	1.99	0.43
3:E:330:ASP:HA	3:E:352:LEU:O	2.17	0.43
6:D:765:GLN:HA	6:D:798:PHE:CE2	2.54	0.43
2:C:917:PRO:HG2	2:C:922:LYS:HE3	2.00	0.43
2:C:1175:VAL:HG11	2:C:1188:PHE:HE1	1.84	0.43
3:E:1093:TRP:NE1	3:E:1105:GLU:OE2	2.43	0.43
3:E:1103:VAL:HG11	3:E:1126:LEU:HD21	2.01	0.43
5:F:925:ILE:HA	5:F:928:TYR:HB3	2.00	0.43
6:D:292:LEU:HA	6:D:295:VAL:HB	1.98	0.43
6:D:306:LYS:O	6:D:306:LYS:NZ	2.52	0.43
6:D:777:ALA:HB3	6:D:785:SER:HB2	2.01	0.43
6:D:1523:GLU:O	6:D:1527:LEU:HG	2.18	0.43
6:D:1579:CYS:HA	6:D:1582:LYS:HD2	2.00	0.43
1:B:22:TRP:CZ2	1:B:304:GLU:HG3	2.53	0.43
3:E:1107:LEU:HG	3:E:1122:ILE:HG21	2.00	0.43
6:D:1145:TYR:CD2	6:D:1154:ALA:HB2	2.54	0.43
1:B:928:ALA:O	1:B:932:LYS:HG2	2.19	0.43
2:C:884:LEU:HD23	2:C:884:LEU:HA	1.86	0.43
3:E:252:GLU:N	3:E:252:GLU:OE1	2.52	0.43
3:E:1179:PHE:O	3:E:1182:GLN:HB2	2.18	0.43
6:D:757:ALA:HA	6:D:766:ILE:HD11	2.00	0.43
6:D:805:GLN:HA	6:D:808:LYS:HD2	2.01	0.43
4:A:171:ARG:HH11	6:D:1322:PRO:HA	1.84	0.43
5:F:161:PRO:HD3	5:F:181:VAL:HG22	1.99	0.43
6:D:1617:ARG:O	6:D:1617:ARG:NE	2.52	0.43
2:C:157:MET:HB2	2:C:163:MET:HE1	2.00	0.43
3:E:837:LYS:HB3	3:E:840:GLY:HA3	2.01	0.43
5:F:348:LEU:HD11	5:F:386:ASP:HB3	2.01	0.43
5:F:822:SER:O	5:F:826:SER:OG	2.26	0.43
1:B:5:LEU:HD23	1:B:5:LEU:HA	1.89	0.42
1:B:376:ASP:OD1	1:B:376:ASP:N	2.52	0.42
1:B:1016:LEU:HD11	1:B:1045:VAL:HG11	2.01	0.42
2:C:569:TYR:HB3	2:C:578:ALA:HB2	1.99	0.42
5:F:574:LEU:HD23	5:F:574:LEU:HA	1.73	0.42
1:B:835:LEU:O	1:B:839:LEU:HG	2.19	0.42
2:C:381:LEU:HD13	2:C:419:MET:HB2	2.01	0.42
2:C:393:ASN:O	2:C:396:ARG:HG3	2.18	0.42
2:C:1232:CYS:SG	2:C:1244:TYR:OH	2.64	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:533:PHE:CG	5:F:573:VAL:HB	2.53	0.42
6:D:836:SER:HA	6:D:839:GLU:HG2	2.00	0.42
6:D:1135:ALA:HB2	6:D:1168:HIS:CE1	2.47	0.42
6:D:1193:GLU:O	6:D:1197:ALA:N	2.44	0.42
1:B:353:TRP:NE1	1:B:358:ASN:HA	2.28	0.42
1:B:532:ASN:OD1	1:B:537:GLN:N	2.39	0.42
1:B:577:ASN:ND2	1:B:614:LEU:H	2.17	0.42
2:C:350:GLU:OE2	2:C:376:ARG:NH2	2.53	0.42
2:C:909:GLY:HA3	2:C:1211:GLY:HA3	2.01	0.42
2:C:951:GLN:NE2	3:E:1031:THR:O	2.53	0.42
3:E:456:ARG:HB2	3:E:824:VAL:HG13	2.00	0.42
5:F:25:PRO:HG3	5:F:106:GLN:HE22	1.84	0.42
6:D:586:VAL:O	6:D:590:LYS:N	2.38	0.42
1:B:118:ASN:CG	1:B:123:LYS:H	2.26	0.42
1:B:212:ARG:CZ	1:B:346:VAL:HA	2.50	0.42
2:C:121:ASP:OD1	2:C:121:ASP:N	2.51	0.42
2:C:312:MET:HE2	2:C:312:MET:HB2	1.76	0.42
2:C:1226:ASP:OD1	2:C:1226:ASP:N	2.51	0.42
3:E:165:LYS:HE3	3:E:172:VAL:HG11	2.01	0.42
4:A:199:LEU:HA	4:A:202:LEU:HG	2.00	0.42
5:F:372:LEU:HD13	5:F:372:LEU:HA	1.83	0.42
5:F:600:SER:HA	5:F:699:MET:HA	2.02	0.42
6:D:508:SER:HB2	6:D:534:ALA:HB2	2.02	0.42
1:B:80:LEU:HB3	1:B:92:TRP:HB2	2.00	0.42
1:B:614:LEU:HD12	1:B:614:LEU:HA	1.87	0.42
1:B:1027:ASP:OD1	1:B:1027:ASP:N	2.48	0.42
3:E:357:LEU:HD12	3:E:368:VAL:HA	2.00	0.42
3:E:911:SER:OG	3:E:912:GLY:N	2.52	0.42
3:E:1011:GLU:OE2	3:E:1035:ARG:NH1	2.37	0.42
6:D:1150:ARG:O	6:D:1150:ARG:NH1	2.46	0.42
2:C:238:ILE:HG23	2:C:250:PHE:HB2	2.02	0.42
2:C:954:PRO:HB2	3:E:1099:ARG:HH11	1.84	0.42
3:E:304:SER:HG	3:E:307:THR:HG1	1.56	0.42
3:E:346:LEU:HD23	3:E:346:LEU:H	1.85	0.42
6:D:1562:GLU:HA	6:D:1565:LEU:HD12	2.00	0.42
1:B:351:MET:HE3	1:B:351:MET:HB3	1.81	0.42
2:C:2:HIS:HE1	2:C:4:SER:HB2	1.84	0.42
2:C:556:MET:HB2	2:C:556:MET:HE2	1.79	0.42
3:E:1081:THR:O	3:E:1085:GLN:NE2	2.35	0.42
6:D:534:ALA:HA	6:D:537:ALA:HB3	2.02	0.42
1:B:3:VAL:HG21	1:B:280:PHE:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:THR:OG1	1:B:172:GLU:N	2.50	0.42
2:C:146:TRP:CE2	2:C:153:LEU:HD13	2.54	0.42
2:C:309:ARG:HD3	2:C:334:VAL:HG13	2.02	0.42
3:E:541:ILE:HG12	3:E:550:PHE:CD1	2.54	0.42
3:E:547:ARG:NE	3:E:560:GLN:HA	2.32	0.42
3:E:574:ASP:O	3:E:580:LEU:HA	2.20	0.42
6:D:1012:ARG:HH21	6:D:1016:HIS:CD2	2.37	0.42
6:D:1345:LEU:HD21	6:D:1452:ILE:HG13	2.02	0.42
1:B:699:ILE:HD12	1:B:699:ILE:HA	1.93	0.42
1:B:1059:GLU:OE2	1:B:1149:ARG:NH2	2.53	0.42
2:C:909:GLY:HA2	2:C:1213:LEU:HG	2.02	0.42
2:C:1019:MET:HB3	2:C:1019:MET:HE3	1.83	0.42
3:E:112:VAL:HA	3:E:115:ILE:HG12	2.01	0.42
3:E:313:MET:HE1	3:E:327:SER:HA	2.01	0.42
3:E:510:PHE:HE1	3:E:526:VAL:HG23	1.85	0.42
3:E:808:LEU:HD23	3:E:808:LEU:HA	1.82	0.42
3:E:1231:LEU:HD13	3:E:1231:LEU:HA	1.86	0.42
6:D:558:ALA:HA	6:D:561:ALA:HB3	2.02	0.42
6:D:972:LEU:HB2	6:D:999:ALA:HB2	2.01	0.42
6:D:1221:ASN:N	6:D:1221:ASN:OD1	2.52	0.42
1:B:118:ASN:HD21	1:B:122:THR:H	1.67	0.42
2:C:305:GLN:NE2	2:C:339:THR:HG21	2.34	0.42
6:D:404:LEU:HD13	6:D:440:GLY:HA2	2.02	0.42
6:D:523:GLU:HB3	6:D:526:ALA:HB3	2.02	0.42
6:D:1005:THR:O	6:D:1009:LEU:HG	2.19	0.42
6:D:1573:HIS:CD2	6:D:1601:ASN:HA	2.51	0.42
1:B:1174:CYS:N	1:B:1179:SER:O	2.50	0.41
2:C:593:MET:HE3	2:C:593:MET:HB3	1.91	0.41
2:C:626:LEU:O	2:C:629:ARG:NH2	2.53	0.41
5:F:116:LYS:HA	5:F:140:ARG:HA	2.02	0.41
5:F:796:LEU:HD12	5:F:805:ALA:HB2	2.02	0.41
6:D:1511:ILE:HA	6:D:1514:LEU:HD12	2.01	0.41
2:C:249:LEU:HD12	2:C:249:LEU:HA	1.90	0.41
3:E:501:ALA:HB2	3:E:535:ILE:HD12	2.02	0.41
1:B:484:ASN:OD1	1:B:484:ASN:N	2.53	0.41
3:E:711:GLU:HG3	3:E:828:ILE:HD12	2.00	0.41
6:D:331:ARG:O	6:D:335:GLN:HG2	2.20	0.41
6:D:607:GLU:HA	6:D:610:LEU:HD23	2.02	0.41
6:D:777:ALA:O	6:D:781:ASP:N	2.47	0.41
3:E:1030:SER:HB2	3:E:1088:GLU:HB2	2.02	0.41
5:F:707:ARG:O	5:F:707:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1235:LEU:HD12	6:D:1236:PRO:HA	2.02	0.41
3:E:467:ILE:HD12	3:E:845:ALA:HB1	2.02	0.41
5:F:502:LEU:HD12	5:F:511:VAL:HG22	2.03	0.41
5:F:799:ARG:HA	5:F:799:ARG:HD3	1.84	0.41
6:D:1433:LEU:HD22	6:D:1434:GLN:HE21	1.86	0.41
6:D:1625:TYR:HA	6:D:1626:PRO:HD3	1.94	0.41
1:B:1149:ARG:HA	1:B:1150:PRO:HD3	1.95	0.41
4:A:196:GLU:HB2	4:A:197:MET:HE2	2.01	0.41
6:D:1353:LEU:HD23	6:D:1353:LEU:HA	1.83	0.41
6:D:510:LEU:HD13	6:D:510:LEU:HA	1.91	0.41
1:B:872:VAL:HG13	1:B:874:MET:HG2	2.01	0.41
2:C:397:ILE:HD13	2:C:410:TRP:HB2	2.03	0.41
3:E:222:ASP:HB3	3:E:223:ASP:H	1.65	0.41
3:E:638:LEU:HB3	3:E:639:GLU:H	1.61	0.41
3:E:668:THR:O	3:E:685:PHE:N	2.37	0.41
6:D:376:ALA:O	6:D:380:ARG:HG2	2.21	0.41
6:D:1228:ARG:H	6:D:1228:ARG:HG3	1.68	0.41
6:D:1260:ASP:OD1	6:D:1261:LEU:N	2.41	0.41
1:B:538:LEU:HD21	1:B:540:VAL:HG23	2.03	0.41
1:B:688:GLN:HG3	1:B:688:GLN:H	1.77	0.41
1:B:763:VAL:HA	1:B:766:VAL:HG12	2.03	0.41
1:B:1049:GLY:O	1:B:1052:SER:OG	2.29	0.41
2:C:483:VAL:HG13	2:C:494:PHE:H	1.86	0.41
2:C:714:LEU:HB3	2:C:716:MET:SD	2.61	0.41
2:C:837:LEU:HD23	2:C:837:LEU:HA	1.93	0.41
2:C:964:ALA:HB1	2:C:989:LEU:HB2	2.03	0.41
2:C:1038:ASP:OD1	2:C:1038:ASP:N	2.54	0.41
3:E:528:THR:OG1	3:E:543:VAL:O	2.32	0.41
3:E:971:TYR:CE2	3:E:994:PHE:HB3	2.56	0.41
4:A:198:LEU:O	4:A:201:GLN:HG2	2.21	0.41
5:F:491:LEU:HA	5:F:505:THR:HA	2.02	0.41
6:D:1211:TYR:OH	6:D:1518:GLU:OE2	2.29	0.41
6:D:1612:ILE:O	6:D:1616:LYS:HG2	2.21	0.41
2:C:350:GLU:HG3	2:C:376:ARG:HE	1.86	0.41
2:C:879:ARG:HH12	3:E:969:LYS:HE2	1.86	0.41
2:C:1035:LYS:HA	2:C:1035:LYS:HD2	1.86	0.41
3:E:188:VAL:HG21	3:E:228:LEU:HD23	2.02	0.41
3:E:1212:LYS:HE3	3:E:1212:LYS:HB3	1.76	0.41
6:D:405:VAL:HG13	6:D:553:TYR:HD2	1.86	0.41
6:D:1141:LEU:HD23	6:D:1141:LEU:HA	1.76	0.41
6:D:1169:TYR:O	6:D:1173:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:THR:HG22	2:C:97:GLN:HB3	2.03	0.40
2:C:903:HIS:NE2	2:C:1257:CYS:O	2.41	0.40
2:C:951:GLN:HB3	2:C:953:LEU:HD13	2.02	0.40
2:C:1270:LYS:H	2:C:1270:LYS:HG3	1.66	0.40
3:E:1051:MET:HG2	3:E:1109:PHE:HZ	1.86	0.40
5:F:501:PHE:HB2	5:F:514:LEU:HD21	2.04	0.40
6:D:740:GLN:HB2	6:D:749:ALA:HB2	2.03	0.40
6:D:960:GLU:O	6:D:963:ASN:HB2	2.21	0.40
6:D:1106:GLN:HB3	6:D:1110:ARG:CZ	2.50	0.40
1:B:45:GLY:O	1:B:50:GLN:NE2	2.37	0.40
2:C:516:THR:OG1	2:C:518:ASP:OD1	2.29	0.40
2:C:692:ASN:OD1	2:C:693:ASP:N	2.54	0.40
3:E:940:TYR:HD2	3:E:946:VAL:HG21	1.86	0.40
6:D:415:ASP:OD1	6:D:415:ASP:N	2.53	0.40
6:D:438:LEU:HD23	6:D:438:LEU:HA	1.94	0.40
6:D:641:PRO:HD3	6:D:670:LEU:HD21	2.03	0.40
6:D:811:LEU:HG	6:D:812:THR:HG23	2.04	0.40
6:D:1440:PRO:HB3	6:D:1466:LEU:HD11	2.03	0.40
1:B:175:VAL:HG21	1:B:234:ILE:HD12	2.03	0.40
1:B:399:ILE:HG23	2:C:587:ALA:HA	2.03	0.40
2:C:6:ARG:NH1	2:C:47:SER:O	2.37	0.40
2:C:696:ARG:HG2	2:C:699:MET:HE2	2.04	0.40
2:C:1027:LEU:HD21	5:F:556:VAL:HA	2.04	0.40
3:E:564:THR:N	3:E:567:GLU:OE1	2.44	0.40
6:D:493:LEU:HD13	6:D:493:LEU:HA	1.97	0.40
6:D:891:TYR:HD1	6:D:891:TYR:HA	1.74	0.40
6:D:1628:ILE:HD13	6:D:1628:ILE:HA	1.96	0.40
1:B:177:ASP:HB2	1:B:184:LEU:HD11	2.02	0.40
1:B:276:ILE:HD12	1:B:298:CYS:HB3	2.03	0.40
1:B:1223:GLU:HA	1:B:1226:VAL:HG12	2.03	0.40
2:C:563:ALA:HA	2:C:566:LEU:HB3	2.04	0.40
2:C:1014:LEU:HD13	2:C:1022:VAL:HG21	2.02	0.40
3:E:314:SER:OG	3:E:326:GLY:O	2.39	0.40
5:F:594:PHE:CZ	5:F:608:SER:HB3	2.57	0.40
5:F:764:ARG:HD3	5:F:764:ARG:HA	1.94	0.40
5:F:766:ASP:N	5:F:766:ASP:OD1	2.52	0.40
6:D:594:HIS:CE1	6:D:595:LEU:HG	2.57	0.40
6:D:761:ARG:HD2	6:D:761:ARG:HA	1.90	0.40
6:D:1162:LEU:HD23	6:D:1162:LEU:HA	1.89	0.40
6:D:1607:GLN:HB2	6:D:1610:LYS:NZ	2.36	0.40
1:B:73:TRP:CH2	1:B:80:LEU:HD12	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:PHE:HA	1:B:859:ALA:HB3	2.04	0.40
2:C:457:THR:OG1	2:C:458:ALA:N	2.55	0.40
2:C:800:LYS:HA	2:C:800:LYS:HD3	1.89	0.40
2:C:1232:CYS:SG	2:C:1254:CYS:HB2	2.61	0.40
3:E:3:LEU:HG	3:E:454:ARG:HG2	2.04	0.40
3:E:1194:LEU:HD21	3:E:1218:VAL:HG11	2.03	0.40
5:F:841:GLN:HG2	5:F:868:PHE:CD1	2.57	0.40
6:D:733:TYR:OH	6:D:753:LEU:HA	2.22	0.40
6:D:835:GLN:H	6:D:835:GLN:HG3	1.69	0.40
6:D:1591:ASP:OD2	6:D:1593:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	1126/1247 (90%)	1091 (97%)	35 (3%)	0	100	100
2	C	1173/1292 (91%)	1119 (95%)	54 (5%)	0	100	100
3	E	1064/1654 (64%)	1023 (96%)	41 (4%)	0	100	100
4	A	51/368 (14%)	45 (88%)	6 (12%)	0	100	100
5	F	907/1376 (66%)	865 (95%)	42 (5%)	0	100	100
6	D	1164/1642 (71%)	1118 (96%)	46 (4%)	0	100	100
All	All	5485/7579 (72%)	5261 (96%)	224 (4%)	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	B	960/1046 (92%)	934 (97%)	26 (3%)	39	62
2	C	1014/1094 (93%)	988 (97%)	26 (3%)	40	62
3	E	903/1373 (66%)	864 (96%)	39 (4%)	26	51
4	A	50/288 (17%)	47 (94%)	3 (6%)	17	44
5	F	779/1177 (66%)	762 (98%)	17 (2%)	45	65
6	D	971/1320 (74%)	916 (94%)	55 (6%)	18	45
All	All	4677/6298 (74%)	4511 (96%)	166 (4%)	32	57

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	SER
1	B	112	VAL
1	B	163	SER
1	B	277	VAL
1	B	310	VAL
1	B	382	SER
1	B	388	GLN
1	B	399	ILE
1	B	415	TYR
1	B	483	THR
1	B	511	LEU
1	B	522	LEU
1	B	578	LEU
1	B	590	VAL
1	B	624	THR
1	B	680	LEU
1	B	720	LYS
1	B	874	MET
1	B	907	LEU
1	B	927	LEU
1	B	948	LEU
1	B	999	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1044	LEU
1	B	1047	ASN
1	B	1172	VAL
1	B	1200	VAL
2	C	94	VAL
2	C	247	VAL
2	C	298	VAL
2	C	305	GLN
2	C	312	MET
2	C	322	VAL
2	C	334	VAL
2	C	353	ILE
2	C	369	ASP
2	C	432	LEU
2	C	435	LEU
2	C	474	VAL
2	C	475	ILE
2	C	481	LEU
2	C	483	VAL
2	C	512	ILE
2	C	539	VAL
2	C	550	LEU
2	C	558	LEU
2	C	620	VAL
2	C	716	MET
2	C	748	VAL
2	C	902	ILE
2	C	908	TYR
2	C	999	VAL
2	C	1096	ARG
3	E	7	ASN
3	E	41	ILE
3	E	42	THR
3	E	50	THR
3	E	66	THR
3	E	68	LEU
3	E	147	LEU
3	E	150	VAL
3	E	224	ILE
3	E	248	VAL
3	E	277	VAL
3	E	322	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	325	PHE
3	E	352	LEU
3	E	381	HIS
3	E	436	ASP
3	E	437	VAL
3	E	446	LEU
3	E	482	CYS
3	E	499	ASN
3	E	500	ILE
3	E	523	ILE
3	E	541	ILE
3	E	548	ILE
3	E	575	ILE
3	E	582	VAL
3	E	591	LEU
3	E	916	VAL
3	E	964	LEU
3	E	970	ARG
3	E	1040	THR
3	E	1049	LEU
3	E	1090	LEU
3	E	1165	ASP
3	E	1174	VAL
3	E	1212	LYS
3	E	1224	MET
3	E	1231	LEU
3	E	1234	GLU
4	A	191	VAL
4	A	199	LEU
4	A	200	VAL
5	F	30	ILE
5	F	185	VAL
5	F	329	GLN
5	F	372	LEU
5	F	401	VAL
5	F	522	THR
5	F	613	ASP
5	F	661	THR
5	F	678	TRP
5	F	690	GLU
5	F	702	VAL
5	F	766	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	788	ILE
5	F	806	LEU
5	F	814	ARG
5	F	833	GLU
5	F	839	CYS
6	D	339	TRP
6	D	400	HIS
6	D	439	CYS
6	D	469	ASP
6	D	474	THR
6	D	510	LEU
6	D	610	LEU
6	D	618	VAL
6	D	622	VAL
6	D	644	PHE
6	D	657	THR
6	D	670	LEU
6	D	679	LEU
6	D	682	LEU
6	D	751	GLU
6	D	847	ILE
6	D	893	ASP
6	D	905	ARG
6	D	918	ILE
6	D	957	THR
6	D	971	VAL
6	D	979	VAL
6	D	994	ASN
6	D	1000	LEU
6	D	1003	LEU
6	D	1008	SER
6	D	1029	GLU
6	D	1045	CYS
6	D	1059	MET
6	D	1098	GLU
6	D	1118	GLU
6	D	1139	ILE
6	D	1156	ASN
6	D	1158	PHE
6	D	1165	THR
6	D	1172	LEU
6	D	1189	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	1221	ASN
6	D	1227	LEU
6	D	1253	TYR
6	D	1257	THR
6	D	1307	LEU
6	D	1327	GLU
6	D	1354	GLU
6	D	1356	ILE
6	D	1431	PHE
6	D	1439	HIS
6	D	1472	ILE
6	D	1473	THR
6	D	1539	LEU
6	D	1551	SER
6	D	1591	ASP
6	D	1593	ASP
6	D	1624	THR
6	D	1634	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	GLN
1	B	106	ASN
1	B	108	ASN
1	B	176	HIS
1	B	229	GLN
1	B	356	ASN
1	B	510	GLN
1	B	684	HIS
1	B	791	GLN
1	B	824	GLN
1	B	1006	GLN
1	B	1047	ASN
2	C	255	ASN
2	C	564	HIS
2	C	769	GLN
2	C	1021	GLN
2	C	1171	GLN
3	E	11	HIS
3	E	14	GLN
3	E	183	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	420	HIS
3	E	481	GLN
3	E	485	GLN
3	E	507	GLN
3	E	554	GLN
5	F	106	GLN
5	F	329	GLN
5	F	349	ASN
5	F	519	GLN
5	F	663	ASN
5	F	669	ASN
5	F	726	HIS
5	F	794	GLN
6	D	308	GLN
6	D	347	HIS
6	D	356	ASN
6	D	490	GLN
6	D	511	ASN
6	D	540	GLN
6	D	649	GLN
6	D	1119	GLN
6	D	1168	HIS
6	D	1578	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28866. These allow visual inspection of the internal detail of the map and identification of artifacts.

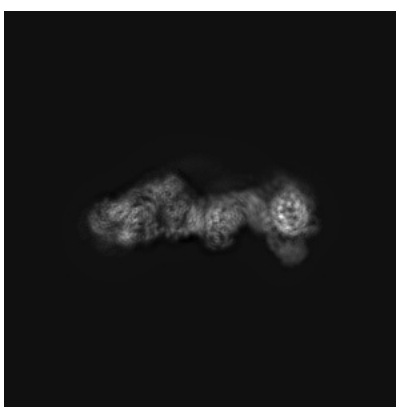
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

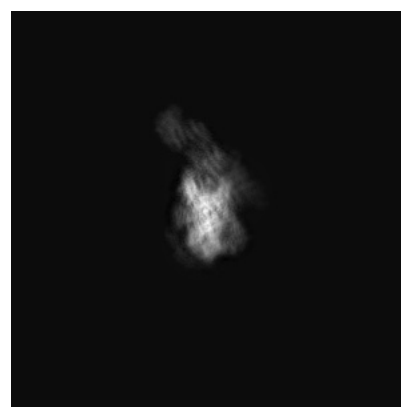
6.1.1 Primary map



X



Y

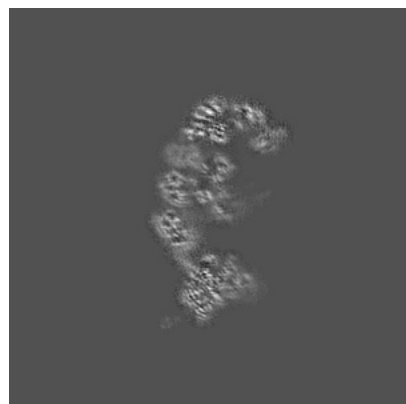


Z

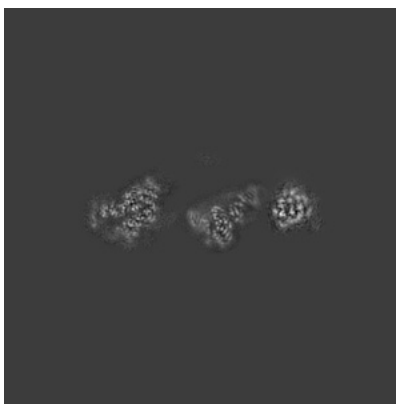
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

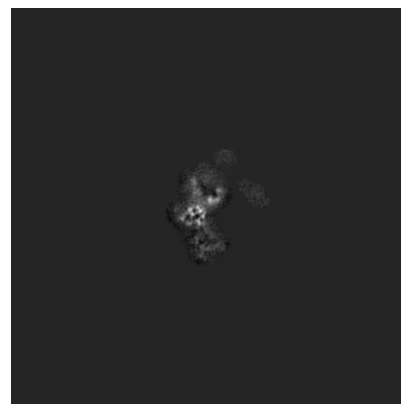
6.2.1 Primary map



X Index: 310



Y Index: 310

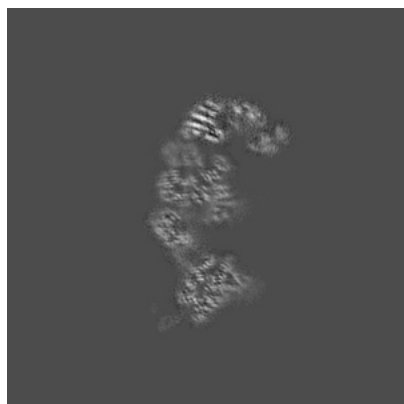


Z Index: 310

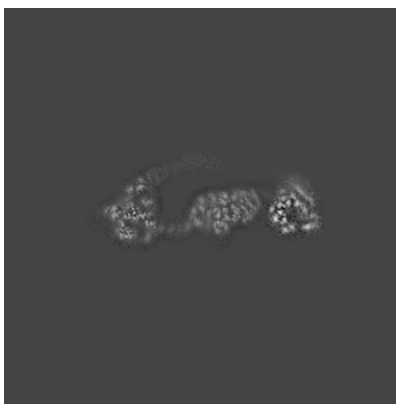
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

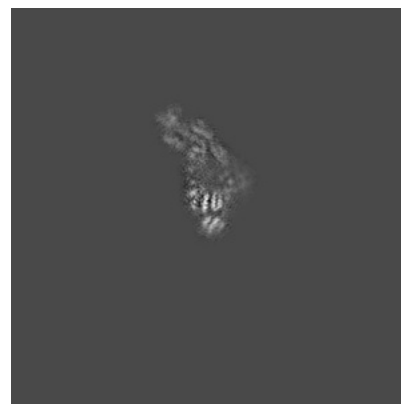
6.3.1 Primary map



X Index: 305



Y Index: 325

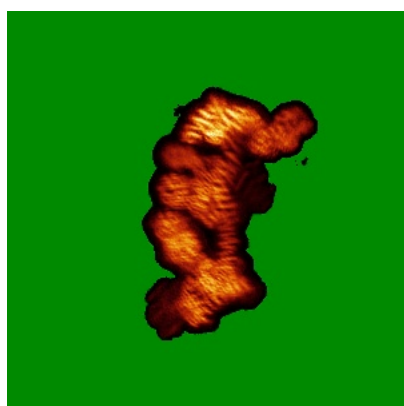


Z Index: 429

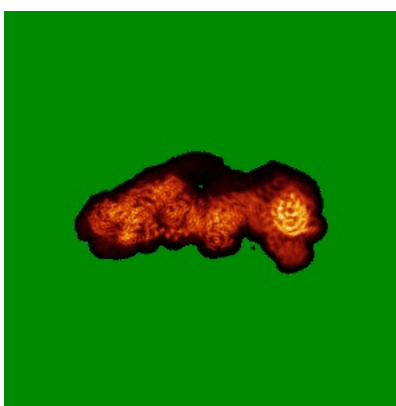
The images above show the largest variance slices of the map in three orthogonal directions.

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

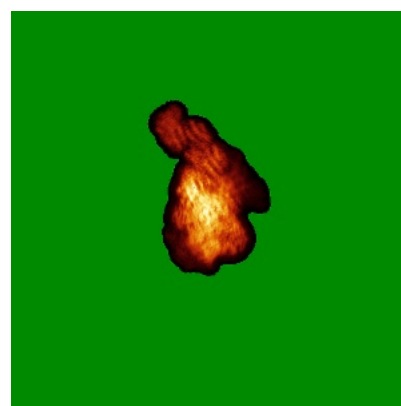
6.4.1 Primary map



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

This section was not generated.

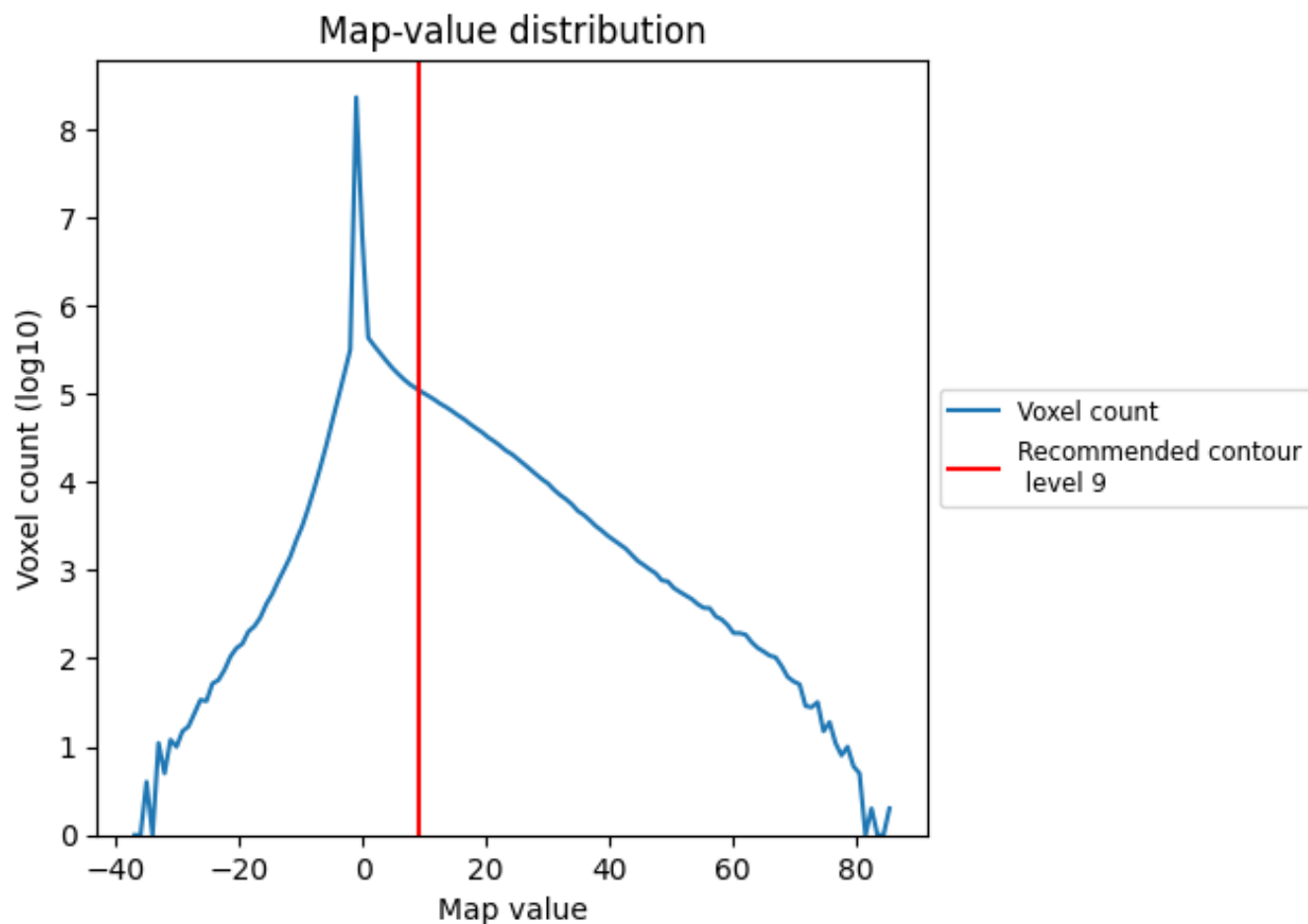
6.6 Mask visualisation

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

7 Map analysis [i](#)

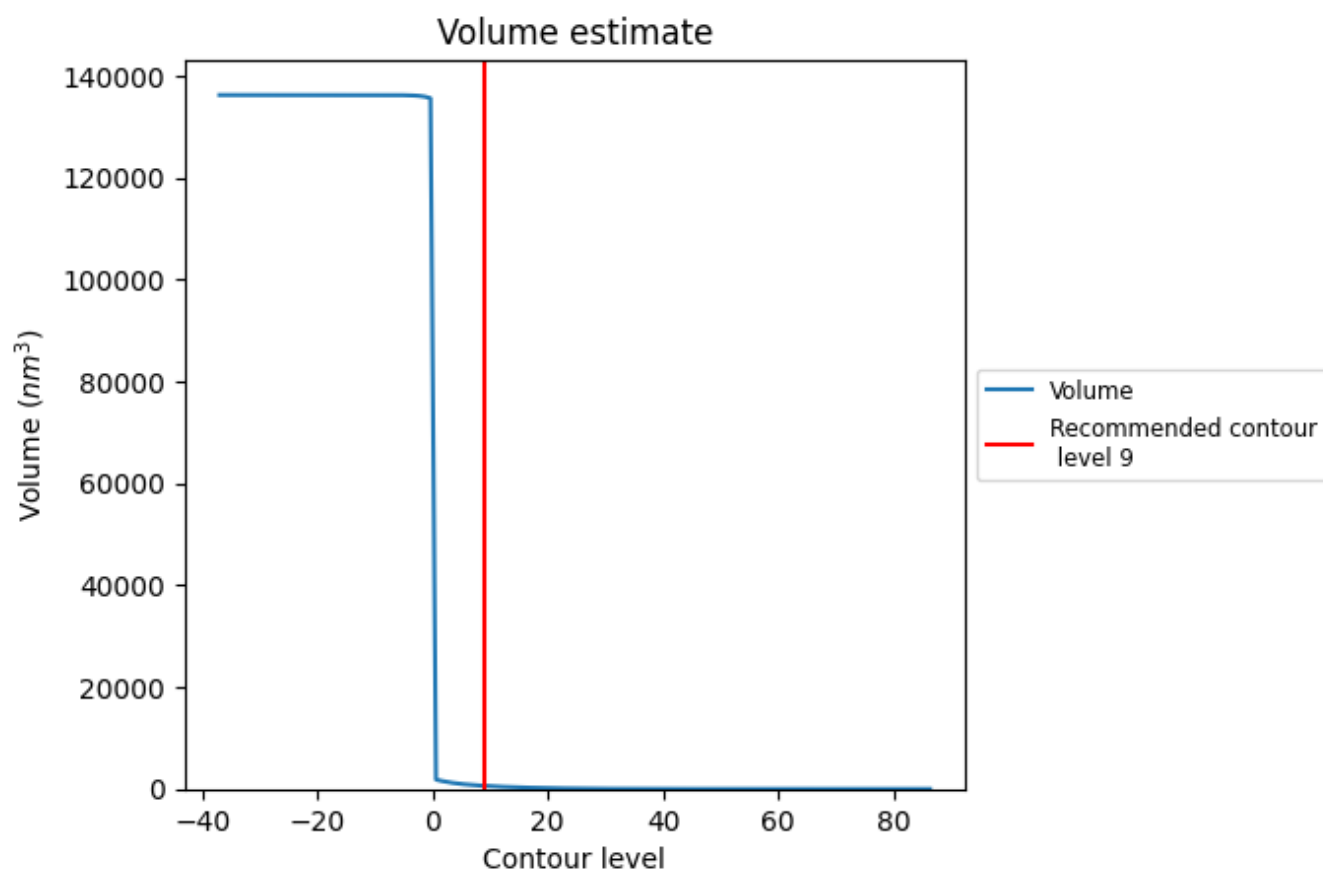
This section contains the results of statistical analysis of the map.

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.

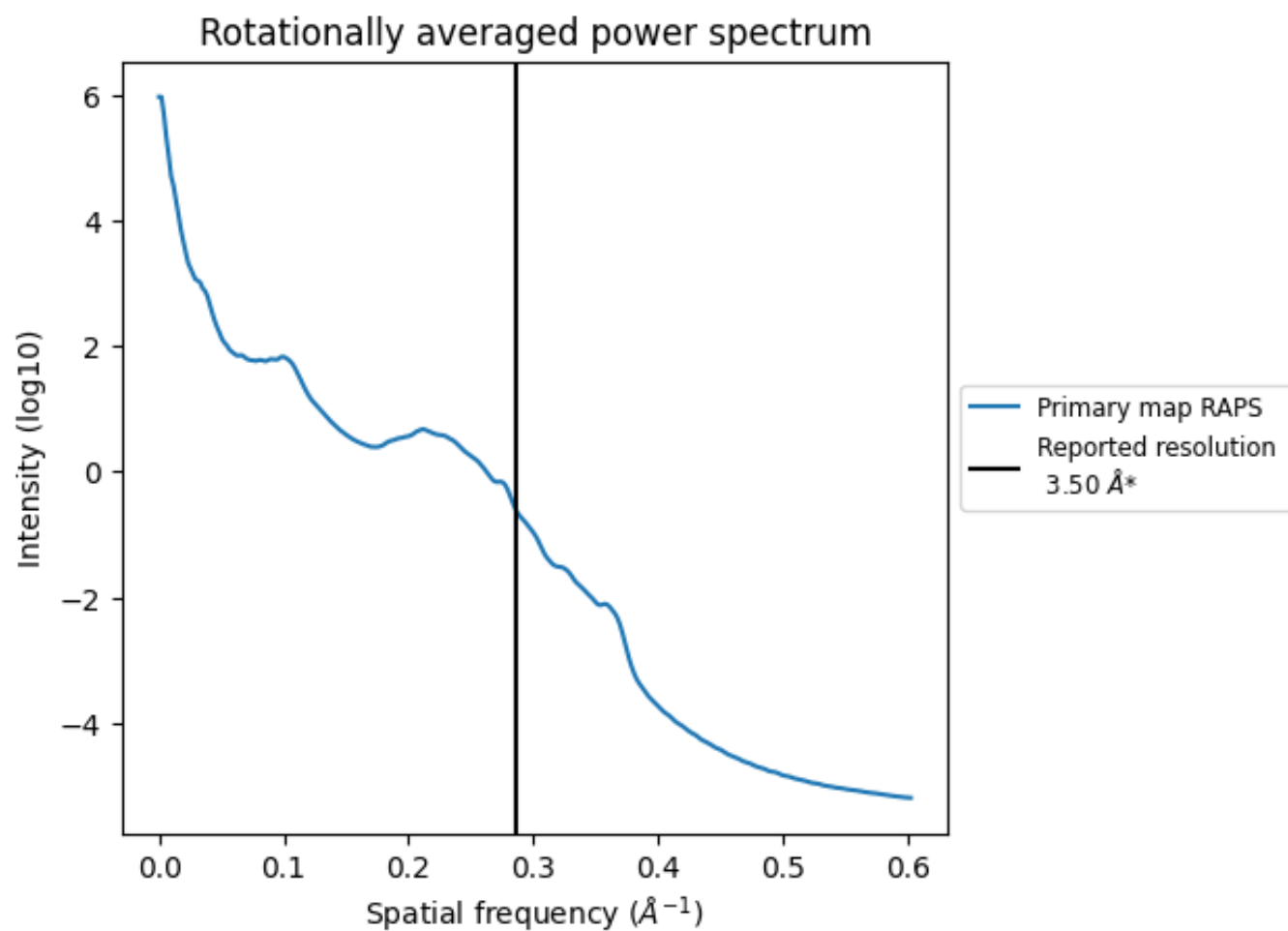
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 619 nm^3 ; this corresponds to an approximate mass of 559 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 0.286 Å⁻¹

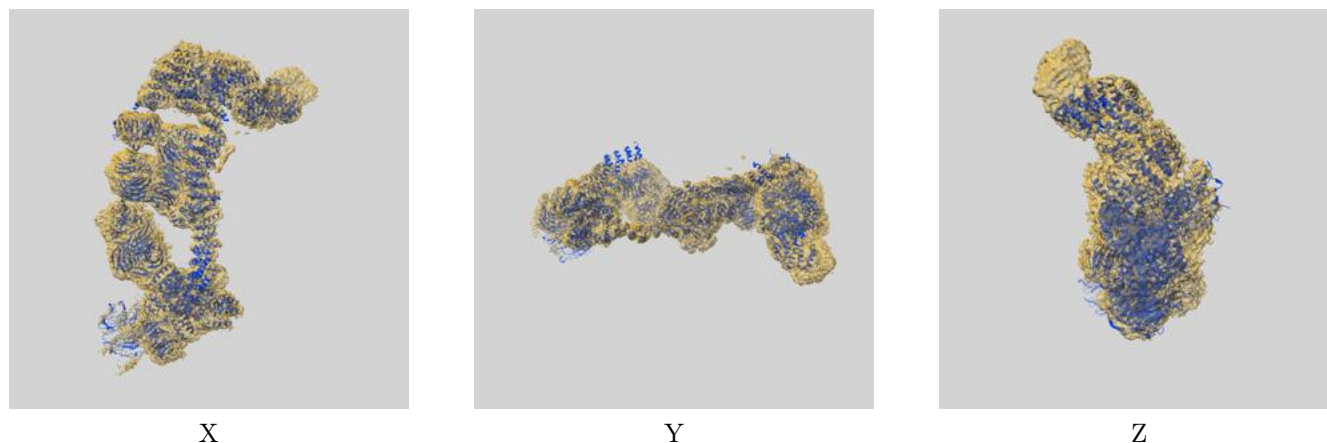
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

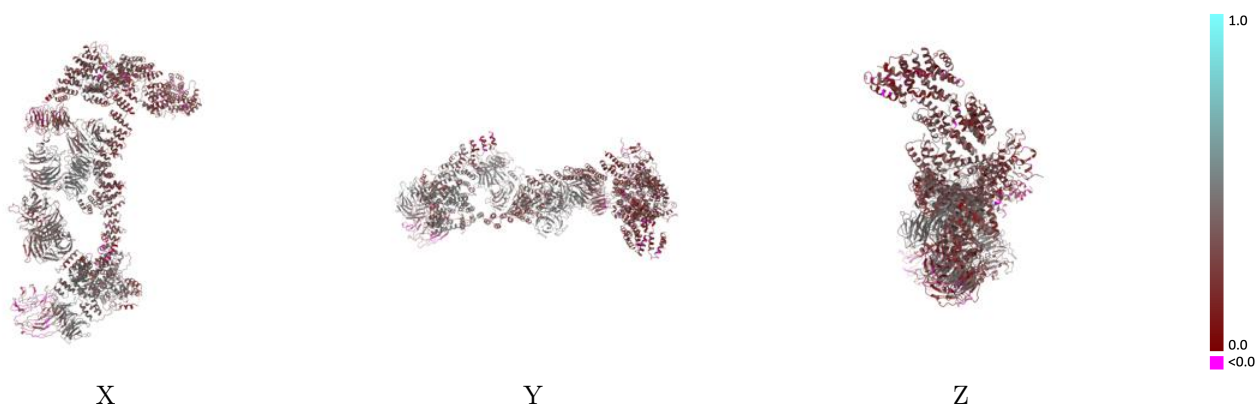
This section contains information regarding the fit between EMDB map EMD-28866 and PDB model 8F5O. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



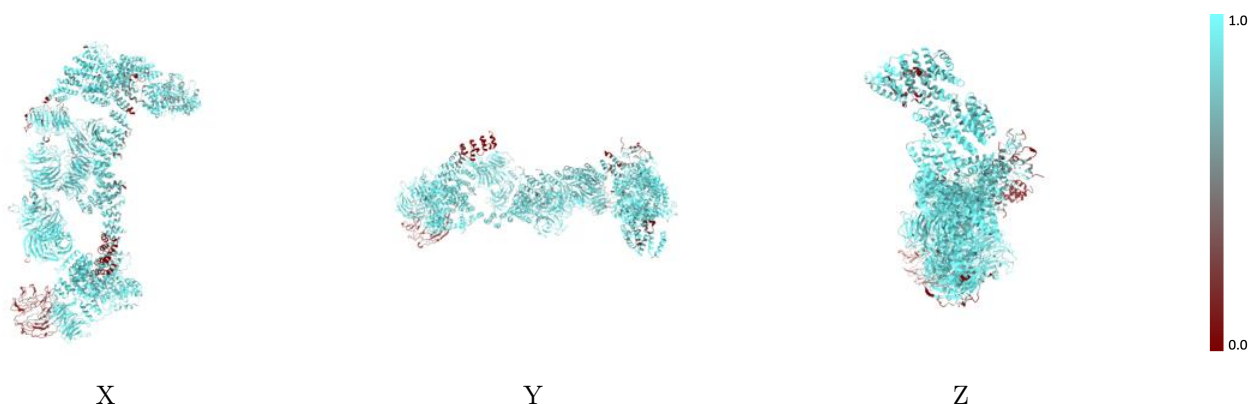
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



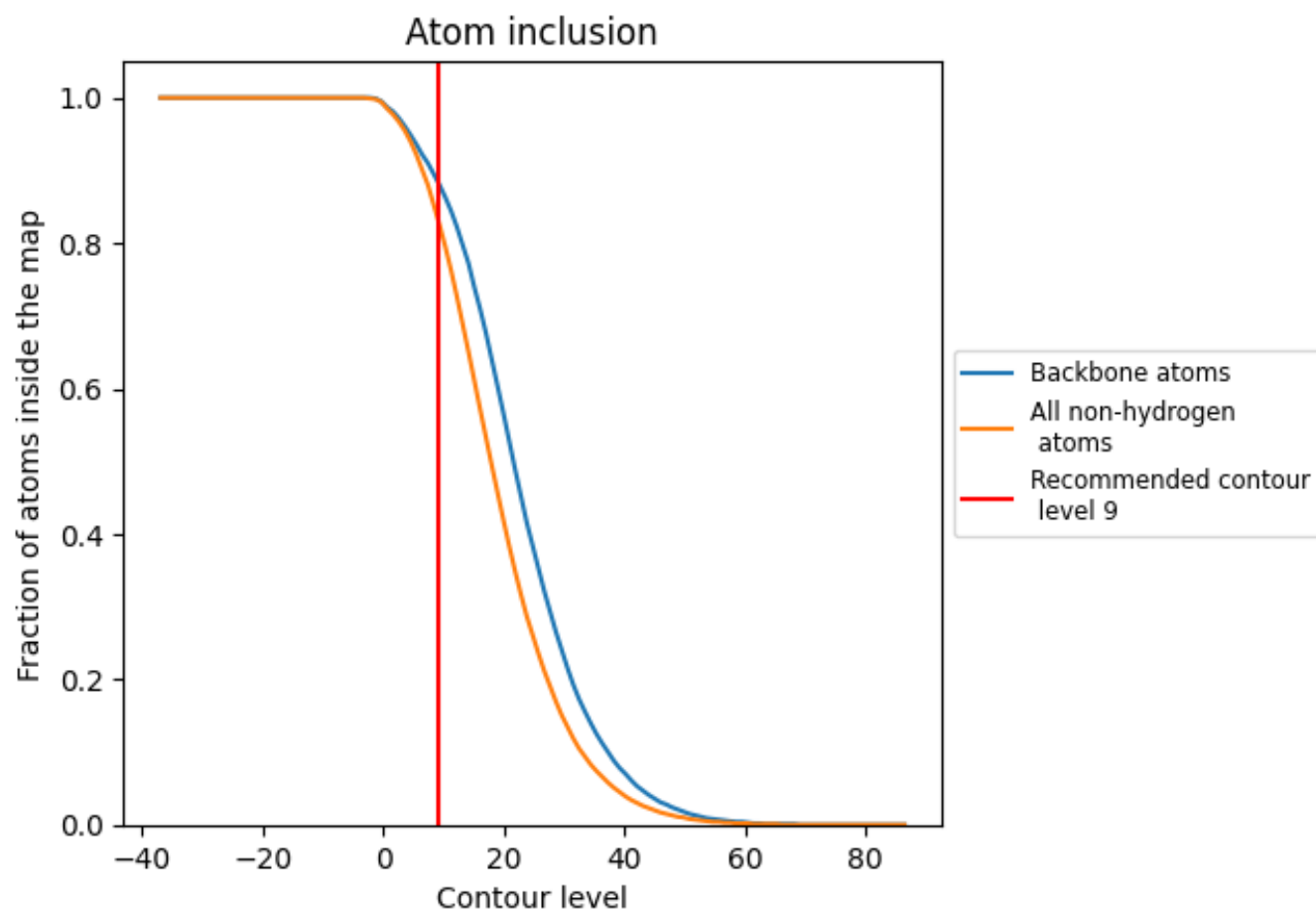
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.3350
A	0.8160	0.2460
B	0.8770	0.3710
C	0.8760	0.3370
D	0.8970	0.2880
E	0.9350	0.3800
F	0.5230	0.2970

