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PDB ID	:	8BJA
EMDB ID	:	EMD-16087
Title	:	Structure of the human UBR5 Dimer.
Authors	:	Hodakova, Z.; Grishkovskaya, I.; Haselbach, D.
Deposited on	:	2022-11-03
Resolution	:	3.00 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 (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:

:	0.0.1. dev 50
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.35
	: : : : :

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 3.00 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.



Motrie	Whole archive	EM structures
Wiethic	$(\# {\rm Entries})$	$(\# { m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	А	2830	9%	13%	·	45%
1	В	2830	43%	13%	·	42%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25204 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 E3 ubiquitin-protein ligase UBR5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	В	1638	Total 12897	C 8178	N 2239	0 2384	S 96	0	0
1	А	1563	Total 12301	C 7806	N 2140	O 2265	S 90	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
В	2799	VAL	-	expression tag	UNP O95071
В	2800	GLY	-	expression tag	UNP O95071
В	2801	SER	-	expression tag	UNP O95071
В	2802	ALA	-	expression tag	UNP O95071
В	2803	TRP	-	expression tag	UNP O95071
В	2804	SER	-	expression tag	UNP O95071
В	2805	HIS	-	expression tag	UNP O95071
В	2806	PRO	-	expression tag	UNP O95071
В	2807	GLN	-	expression tag	UNP O95071
В	2808	PHE	-	expression tag	UNP O95071
В	2809	GLU	-	expression tag	UNP O95071
В	2810	LYS	-	expression tag	UNP O95071
В	2811	GLY	-	expression tag	UNP O95071
В	2812	GLY	-	expression tag	UNP O95071
В	2813	GLY	-	expression tag	UNP O95071
В	2814	SER	-	expression tag	UNP O95071
В	2815	GLY	-	expression tag	UNP O95071
В	2816	GLY	-	expression tag	UNP O95071
В	2817	GLY	-	expression tag	UNP O95071
В	2818	SER	-	expression tag	UNP O95071
В	2819	GLY	-	expression tag	UNP O95071
В	2820	GLY	-	expression tag	UNP O95071
В	2821	SER	-	expression tag	UNP O95071
В	2822	ALA	-	expression tag	UNP O95071
В	2823	TRP	-	expression tag	UNP O95071
В	2824	SER	-	expression tag	UNP O95071

There are 64 discrepancies between the modelled and reference sequences:



Continu	Continued from previous page							
Chain	Residue	Modelled	Actual	Comment	Reference			
В	2825	HIS	-	expression tag	UNP O95071			
В	2826	PRO	-	expression tag	UNP O95071			
В	2827	GLN	-	expression tag	UNP O95071			
В	2828	PHE	-	expression tag	UNP O95071			
В	2829	GLU	-	expression tag	UNP O95071			
В	2830	LYS	-	expression tag	UNP O95071			
A	2799	VAL	-	expression tag	UNP O95071			
A	2800	GLY	-	expression tag	UNP O95071			
А	2801	SER	-	expression tag	UNP O95071			
А	2802	ALA	-	expression tag	UNP O95071			
A	2803	TRP	-	expression tag	UNP O95071			
A	2804	SER	-	expression tag	UNP O95071			
А	2805	HIS	-	expression tag	UNP O95071			
А	2806	PRO	-	expression tag	UNP O95071			
А	2807	GLN	-	expression tag	UNP O95071			
A	2808	PHE	-	expression tag	UNP O95071			
А	2809	GLU	-	expression tag	UNP O95071			
А	2810	LYS	-	expression tag	UNP O95071			
А	2811	GLY	-	expression tag	UNP O95071			
A	2812	GLY	-	expression tag	UNP O95071			
A	2813	GLY	-	expression tag	UNP O95071			
A	2814	SER	-	expression tag	UNP O95071			
A	2815	GLY	-	expression tag	UNP O95071			
A	2816	GLY	-	expression tag	UNP O95071			
A	2817	GLY	-	expression tag	UNP O95071			
A	2818	SER	-	expression tag	UNP O95071			
A	2819	GLY	-	expression tag	UNP O95071			
A	2820	GLY	-	expression tag	UNP O95071			
A	2821	SER	-	expression tag	UNP O95071			
A	2822	ALA	-	expression tag	UNP O95071			
A	2823	TRP	-	expression tag	UNP O95071			
A	2824	SER	-	expression tag	UNP O95071			
A	2825	HIS	-	expression tag	UNP O95071			
A	2826	PRO	-	expression tag	UNP O95071			
A	2827	GLN	-	expression tag	UNP 095071			
A	2828	PHE	-	expression tag	UNP 095071			
A	2829	GLU	-	expression tag	UNP O95071			
A	2830	LYS	-	expression tag	UNP O95071			

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• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
2	В	3	Total Zn 3 3	0
2	А	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: E3 ubiquitin-protein ligase UBR5







PROTEIN DATA BANK





















4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288287	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.330	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0632	Depositor
Map size (Å)	446.69998, 446.69998, 446.69998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.489, 1.489, 1.489	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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.29	0/12550	0.55	0/17001	
1	В	0.29	0/13155	0.55	0/17813	
All	All	0.29	0/25705	0.55	0/34814	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	В	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	2266	ARG	Sidechain
1	В	2246	ARG	Sidechain
1	В	2248	ARG	Sidechain

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	12301	0	12343	253	0
1	В	12897	0	12962	251	0
2	А	3	0	0	0	0
2	В	3	0	0	0	0
All	All	25204	0	25305	497	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:2656:LYS:HA	1:A:2659:LEU:HB2	1.54	0.89
1:A:2709:GLN:N	1:A:2709:GLN:HE21	1.71	0.88
1:B:1216:HIS:HD2	1:B:1219:HIS:ND1	1.72	0.85
1:B:1796:SER:HG	1:B:1957:TRP:HD1	1.22	0.84
1:B:1961:MET:HG3	1:B:2171:PRO:HB3	1.60	0.83
1:A:387:LYS:HE2	1:A:387:LYS:H	1.45	0.81
1:A:2542:GLN:O	1:A:2543:ASN:ND2	2.17	0.78
1:A:2749:MET:HG3	1:A:2750:PRO:HD2	1.66	0.77
1:A:1870:HIS:HD2	1:A:1872:LEU:H	1.32	0.77
1:A:752:ASP:OD1	1:A:753:SER:N	2.19	0.76
1:B:1488:MET:HB3	1:A:1841:TRP:HE1	1.52	0.74
1:A:2544:GLU:OE1	1:A:2544:GLU:N	2.21	0.73
1:A:424:ILE:HG22	1:A:438:THR:HG22	1.70	0.73
1:A:1187:GLU:OE1	1:A:1187:GLU:N	2.22	0.72
1:B:2507:GLN:HB3	1:B:2511:ARG:HH22	1.54	0.71
1:B:1248:LYS:HZ1	1:B:1251:ARG:HD3	1.55	0.70
1:B:471:GLU:HB2	1:B:487:LEU:HD13	1.73	0.70
1:A:1199:CYS:SG	1:A:1216:HIS:HE1	2.11	0.70
1:A:909:GLN:OE1	1:A:909:GLN:N	2.21	0.70
1:B:2053:GLN:N	1:B:2053:GLN:OE1	2.25	0.69
1:A:2723:MET:SD	1:A:2723:MET:N	2.60	0.69
1:A:2202:GLU:N	1:A:2202:GLU:OE1	2.24	0.69
1:A:2046:GLU:N	1:A:2046:GLU:OE2	2.26	0.69
1:B:479:CYS:SG	1:B:480:ALA:N	2.65	0.69
1:B:2256:MET:HG2	1:B:2312:LEU:HD22	1.74	0.69
1:B:893:MET:H	1:B:893:MET:HE3	1.57	0.68
1:B:1176:ASN:O	1:B:1251:ARG:NH2	2.27	0.68
1:B:2219:GLU:OE1	1:B:2219:GLU:N	2.26	0.67



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:796:GLU:OE2	1:A:796:GLU:N	2.27	0.67
1:A:2661:VAL:HG12	1:A:2662:LEU:HD22	1.75	0.67
1:A:1326:GLN:OE1	1:A:1326:GLN:N	2.18	0.67
1:A:2182:HIS:ND1	1:A:2184:MET:SD	2.64	0.67
1:B:1822:GLN:N	1:B:1822:GLN:OE1	2.27	0.67
1:B:2277:VAL:HG21	1:B:2538:LEU:HD11	1.77	0.66
1:A:2653:ALA:HA	1:A:2656:LYS:NZ	2.09	0.66
1:B:2202:GLU:N	1:B:2202:GLU:OE2	2.27	0.66
1:B:411:HIS:HB3	1:B:414:ALA:HB2	1.77	0.66
1:A:890:GLN:N	1:A:890:GLN:OE1	2.30	0.65
1:A:61:LEU:HD12	1:A:374:ILE:HG12	1.78	0.65
1:B:893:MET:HA	1:B:896:GLU:HB3	1.79	0.64
1:A:1188:HIS:HB3	1:A:1229:THR:HB	1.78	0.64
1:A:2747:GLN:N	1:A:2747:GLN:OE1	2.30	0.64
1:B:2245:ASP:HB3	1:B:2282:LYS:HB2	1.80	0.64
1:A:916:CYS:SG	1:A:917:ASP:N	2.70	0.64
1:A:2617:LEU:HD23	1:A:2641:HIS:HD2	1.63	0.64
1:A:1104:GLU:N	1:A:1104:GLU:OE2	2.30	0.63
1:A:1248:LYS:HE3	1:A:1248:LYS:HA	1.81	0.63
1:A:2669:ASP:OD1	1:A:2670:LEU:N	2.31	0.63
1:B:2221:LYS:HG2	1:B:2224:LYS:HZ1	1.63	0.63
1:B:1265:VAL:O	1:B:1274:HIS:NE2	2.32	0.62
1:A:2730:VAL:HA	1:A:2733:TRP:HB2	1.82	0.62
1:A:2606:LEU:HD13	1:A:2610:GLU:HG2	1.81	0.62
1:B:463:GLN:OE1	1:B:463:GLN:N	2.32	0.62
1:B:846:MET:HB3	1:B:867:ILE:HG23	1.82	0.62
1:A:765:TRP:O	1:A:767:ARG:NH1	2.32	0.62
1:A:2236:GLN:NE2	1:A:2273:ALA:O	2.32	0.62
1:B:1914:ARG:NH1	1:A:1505:ASP:OD1	2.31	0.61
1:A:2248:ARG:NE	1:A:2307:GLU:OE2	2.32	0.61
1:B:2:THR:HG22	1:B:872:GLU:HA	1.82	0.61
1:A:1213:ARG:HG3	1:A:1213:ARG:HH11	1.66	0.61
1:A:2219:GLU:N	1:A:2219:GLU:OE1	2.33	0.61
1:A:2636:ARG:HG3	1:A:2637:LYS:HD2	1.83	0.61
1:A:880:ILE:HG13	1:A:1088:ILE:HG21	1.83	0.61
1:A:2053:GLN:N	1:A:2053:GLN:OE1	2.33	0.61
1:B:2755:ARG:NH2	1:B:2762:LEU:O	2.33	0.61
1:A:779:GLU:OE1	1:A:779:GLU:N	2.25	0.61
1:B:2098:LEU:HD12	1:B:2099:PRO:HD2	1.82	0.61
1:A:1080:ASP:OD1	1:A:1081:ARG:N	2.33	0.61
1:A:2502:ALA:O	1:A:2525:ARG:NH2	2.33	0.61



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1237:LYS:HE2	1:B:1237:LYS:H	1.66	0.60
1:B:1964:GLN:HB2	1:B:2171:PRO:HG2	1.83	0.60
1:B:2308:LYS:HA	1:B:2308:LYS:HE2	1.82	0.60
1:A:457:LYS:HE3	1:A:457:LYS:HA	1.83	0.60
1:A:440:ASN:OD1	1:A:440:ASN:N	2.35	0.60
1:A:2668:GLU:OE2	1:A:2668:GLU:N	2.23	0.60
1:A:1095:SER:O	1:A:1099:GLN:NE2	2.33	0.60
1:A:2557:VAL:HG11	1:A:2651:LEU:HG	1.82	0.60
1:A:1360:ILE:HG22	1:A:1363:LEU:HD12	1.83	0.59
1:B:2297:THR:HG21	1:B:2736:SER:HA	1.83	0.59
1:A:430:ASN:ND2	1:A:478:CYS:O	2.35	0.59
1:A:2637:LYS:HE2	1:A:2637:LYS:HA	1.84	0.59
1:B:1818:LYS:HD3	1:B:1819:LEU:N	2.17	0.59
1:B:2509:GLY:O	1:B:2511:ARG:NH2	2.31	0.59
1:B:380:GLU:HA	1:B:394:LYS:HA	1.84	0.59
1:B:401:TYR:CE2	1:B:412:PRO:HD3	2.38	0.59
1:B:501:GLN:HA	1:B:504:LYS:HE3	1.84	0.59
1:B:1289:GLU:OE1	1:B:1289:GLU:N	2.34	0.58
1:A:2530:ARG:HH12	1:A:2534:ARG:CZ	2.16	0.58
1:B:1366:GLU:N	1:B:1366:GLU:OE1	2.36	0.58
1:B:1804:LYS:HE2	1:B:1804:LYS:N	2.18	0.58
1:B:2289:SER:OG	1:B:2768:CYS:O	2.21	0.58
1:B:2730:VAL:HA	1:B:2733:TRP:HB2	1.83	0.58
1:A:1920:TYR:HA	1:A:1938:VAL:HG21	1.84	0.58
1:B:2527:ASN:O	1:B:2531:ASN:N	2.34	0.58
1:B:399:GLU:OE2	1:B:402:ARG:HG3	2.02	0.58
1:B:393:TRP:NE1	1:B:398:SER:O	2.28	0.58
1:B:2304:LEU:HG	1:B:2514:TYR:CE2	2.39	0.58
1:A:1369:VAL:O	1:A:1370:TYR:HB2	2.03	0.58
1:B:2731:TYR:HD1	1:B:2735:SER:HA	1.69	0.58
1:A:1512:GLU:OE1	1:A:1512:GLU:N	2.35	0.58
1:B:2502:ALA:O	1:B:2517:ARG:NH2	2.29	0.58
1:A:2656:LYS:H	1:A:2656:LYS:HD3	1.69	0.58
1:B:387:LYS:HE3	1:B:387:LYS:HA	1.86	0.57
1:A:18:LEU:HD11	1:A:811:ILE:HD11	1.86	0.57
1:B:480:ALA:HB2	1:B:806:GLN:HE22	1.70	0.57
1:A:741:PRO:HG2	1:A:744:THR:HG21	1.84	0.57
1:B:890:GLN:NE2	1:B:894:ASN:HD21	2.02	0.57
1:A:2579:LEU:HD21	1:A:2635:VAL:HG22	1.87	0.57
1:A:2276:ARG:NH1	1:A:2276:ARG:HB2	2.19	0.57
1:A:822:MET:HE1	1:A:830:ILE:HG12	1.87	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1:MET:SD	1:B:1:MET:N	2.71	0.57
1:B:411:HIS:HD2	1:B:413:ARG:H	1.53	0.56
1:B:2244:VAL:O	1:B:2282:LYS:N	2.37	0.56
1:B:411:HIS:CD2	1:B:412:PRO:HD2	2.41	0.56
1:B:1392:THR:OG1	1:B:1393:ALA:N	2.36	0.56
1:B:2525:ARG:HG3	1:B:2525:ARG:HH11	1.70	0.56
1:B:2558:LEU:HA	1:B:2655:ARG:HD2	1.87	0.56
1:A:499:PHE:HA	1:A:502:ARG:HB2	1.87	0.56
1:B:1099:GLN:HB3	1:B:1100:PRO:HD3	1.88	0.56
1:A:825:ASP:OD1	1:A:829:GLY:N	2.38	0.56
1:B:411:HIS:CD2	1:B:413:ARG:H	2.24	0.56
1:B:1351:LYS:O	1:B:1351:LYS:NZ	2.31	0.56
1:A:1418:ARG:HG3	1:A:1418:ARG:HH11	1.71	0.56
1:B:397:GLU:N	1:B:397:GLU:OE1	2.37	0.56
1:B:1519:LEU:HD12	1:B:1520:PRO:HD2	1.88	0.56
1:B:1961:MET:HB3	1:B:2173:CYS:SG	2.45	0.56
1:B:900:VAL:HG23	1:B:901:LEU:HG	1.87	0.56
1:B:24:GLU:OE1	1:B:24:GLU:N	2.38	0.56
1:A:24:GLU:HA	1:A:27:GLU:HG3	1.88	0.55
1:B:2558:LEU:HB3	1:B:2658:LEU:HD23	1.89	0.55
1:A:356:LEU:HD13	1:A:357:GLY:N	2.21	0.55
1:B:781:GLU:OE1	1:B:781:GLU:HA	2.07	0.55
1:A:765:TRP:CH2	1:A:767:ARG:HD3	2.41	0.55
1:A:1124:ARG:NE	1:A:1177:ASP:OD1	2.33	0.55
1:A:1334:GLN:HA	1:A:1404:THR:HG21	1.88	0.55
1:B:767:ARG:HD2	1:B:781:GLU:OE2	2.07	0.55
1:B:2174:SER:O	1:B:2174:SER:OG	2.23	0.55
1:A:2721:MET:SD	1:A:2726:ARG:NH1	2.80	0.55
1:A:893:MET:HE3	1:A:893:MET:H	1.72	0.54
1:B:52:VAL:HB	1:B:376:ALA:HB2	1.90	0.54
1:B:1513:LEU:HD13	1:A:1922:LEU:HD22	1.89	0.54
1:A:1870:HIS:CD2	1:A:1872:LEU:H	2.19	0.54
1:B:499:PHE:O	1:B:503:LYS:N	2.40	0.54
1:B:907:MET:SD	1:B:907:MET:N	2.79	0.54
1:B:1399:ASP:OD1	1:B:1462:ARG:NH2	2.39	0.54
1:B:2779:SER:OG	1:B:2781:GLN:OE1	2.25	0.54
1:A:494:TRP:HD1	1:A:735:PRO:HA	1.71	0.54
1:B:780:GLN:N	1:B:780:GLN:OE1	2.41	0.54
1:B:2707:LEU:HD11	1:B:2754:ILE:HD13	1.88	0.54
1:B:832:ASP:N	1:B:832:ASP:OD1	2.41	0.54
1:B:889:ARG:HD3	1:B:890:GLN:N	2.23	0.54



	the page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:898:ALA:O	1:A:904:ASN:ND2	2.41	0.54
1:B:1358:SER:OG	1:B:1359:ARG:N	2.41	0.54
1:A:1804:LYS:HE3	1:A:1804:LYS:HA	1.89	0.54
1:B:2296:TYR:CE2	1:B:2544:GLU:HG3	2.43	0.53
1:A:370:LYS:O	1:A:386:SER:N	2.39	0.53
1:A:461:THR:O	1:A:463:GLN:NE2	2.41	0.53
1:B:907:MET:HA	1:B:910:THR:HG22	1.90	0.53
1:A:844:LEU:HD13	1:A:869:MET:HB3	1.91	0.53
1:B:1108:ALA:O	1:B:1110:ASP:N	2.41	0.53
1:B:2218:PHE:CE1	1:B:2222:GLU:HB3	2.43	0.53
1:A:57:HIS:HB2	1:A:69:ARG:HH21	1.73	0.53
1:A:54:GLY:HA3	1:A:395:TRP:HZ2	1.73	0.53
1:B:874:GLN:HB3	1:B:877:MET:HB3	1.91	0.53
1:B:2676:ARG:NH1	1:B:2676:ARG:HB2	2.24	0.53
1:B:1444:ALA:HB2	1:B:1499:LEU:HB3	1.90	0.53
1:B:367:ASP:N	1:B:367:ASP:OD1	2.42	0.52
1:A:2239:ASP:N	1:A:2239:ASP:OD1	2.41	0.52
1:B:2676:ARG:HB2	1:B:2676:ARG:HH11	1.74	0.52
1:B:502:ARG:O	1:B:505:MET:HG3	2.10	0.52
1:B:2549:THR:HG22	1:B:2680:ASN:HD22	1.74	0.52
1:B:365:ASP:N	1:B:365:ASP:OD1	2.42	0.52
1:B:1290:HIS:CD2	1:B:1321:PRO:HB2	2.45	0.52
1:B:2211:ILE:HD12	1:B:2211:ILE:O	2.09	0.52
1:A:796:GLU:H	1:A:797:ARG:NH2	2.07	0.52
1:B:876:LEU:HD23	1:B:911:PHE:CE1	2.44	0.52
1:B:1236:GLU:HB2	1:B:1237:LYS:NZ	2.23	0.52
1:A:2533:GLY:HA3	1:A:2657:GLY:HA3	1.91	0.52
1:B:2598:MET:HE1	1:B:2600:LEU:HG	1.91	0.52
1:B:507:GLU:N	1:B:507:GLU:OE1	2.43	0.52
1:B:916:CYS:SG	1:B:917:ASP:N	2.80	0.52
1:B:2610:GLU:OE1	1:B:2642:ARG:NH1	2.43	0.52
1:B:2668:GLU:N	1:B:2668:GLU:OE1	2.42	0.52
1:A:2729:LEU:O	1:A:2733:TRP:N	2.40	0.52
1:B:498:PRO:HA	1:B:502:ARG:HB2	1.92	0.52
1:B:886:GLU:OE1	1:B:886:GLU:HA	2.10	0.52
1:A:18:LEU:HD22	1:A:809:PRO:HB2	1.91	0.52
1:A:1083:ALA:O	1:A:1086:HIS:ND1	2.28	0.52
1:B:401:TYR:HE2	1:B:412:PRO:HD3	1.75	0.52
1:B:2687:VAL:HG21	1:B:2719:GLU:HG2	1.91	0.51
1:B:1351:LYS:O	1:B:1521:PRO:HD3	2.10	0.51
1:A:2571:PHE:HE2	1:A:2642:ARG:HE	1.57	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:47:THR:OG1	1:A:63:GLU:OE1	2.28	0.51
1:B:389:GLU:HG2	1:B:391:TYR:HE1	1.76	0.51
1:A:887:ALA:HA	1:A:890:GLN:HE22	1.74	0.51
1:B:1951:PHE:HE2	1:B:2193:LEU:HD21	1.75	0.51
1:B:2721:MET:SD	1:B:2721:MET:N	2.83	0.51
1:B:2114:MET:SD	1:B:2176:MET:HG2	2.51	0.51
1:B:1152:ASP:OD1	1:B:1153:VAL:N	2.44	0.51
1:B:2591:ALA:O	1:B:2595:PHE:N	2.41	0.51
1:A:385:SER:OG	1:A:389:GLU:OE1	2.28	0.51
1:A:765:TRP:CZ2	1:A:767:ARG:HD3	2.46	0.51
1:A:2035:ILE:HG13	1:A:2037:PRO:HD2	1.91	0.51
1:A:2243:GLU:N	1:A:2258:GLN:OE1	2.43	0.51
1:A:2532:ILE:HG13	1:A:2535:ILE:HD11	1.92	0.51
1:B:370:LYS:O	1:B:386:SER:N	2.43	0.50
1:B:1233:ASP:O	1:B:1237:LYS:NZ	2.41	0.50
1:A:1331:ARG:O	1:A:1331:ARG:NH1	2.41	0.50
1:B:2600:LEU:O	1:B:2626:VAL:N	2.45	0.50
1:A:1124:ARG:HH21	1:A:1177:ASP:HA	1.75	0.50
1:B:2052:ASP:HB3	1:B:2053:GLN:OE1	2.11	0.50
1:A:880:ILE:H	1:A:880:ILE:HD12	1.76	0.50
1:A:435:THR:HG23	1:A:445:THR:HB	1.93	0.50
1:A:1836:ILE:O	1:A:1840:ASN:ND2	2.43	0.50
1:B:895:LEU:HD12	1:B:1097:VAL:HG21	1.93	0.50
1:A:40:LEU:C	1:A:42:VAL:H	2.15	0.50
1:A:405:GLN:H	1:A:405:GLN:CD	2.16	0.50
1:A:2257:ARG:O	1:A:2261:ASN:ND2	2.45	0.50
1:A:1958:ILE:O	1:A:1962:ASN:ND2	2.45	0.49
1:A:2653:ALA:HA	1:A:2656:LYS:HZ2	1.75	0.49
1:A:2728:ASP:O	1:A:2732:PHE:N	2.35	0.49
1:B:2046:GLU:N	1:B:2046:GLU:OE1	2.45	0.49
1:A:2251:LEU:O	1:A:2255:THR:OG1	2.25	0.49
1:A:2653:ALA:HA	1:A:2656:LYS:HZ3	1.74	0.49
1:B:468:LEU:HD13	1:B:473:ILE:HD11	1.93	0.49
1:B:2592:ASP:OD1	1:B:2593:ALA:N	2.45	0.49
1:A:2600:LEU:O	1:A:2626:VAL:N	2.35	0.49
1:A:905:LEU:HA	1:A:909:GLN:HE22	1.77	0.49
1:A:1240:CYS:SG	1:A:1242:THR:OG1	2.69	0.49
1:B:1860:ALA:HB2	1:B:1871:PRO:HG2	1.93	0.49
1:B:2542:GLN:HG2	1:B:2544:GLU:OE1	2.12	0.49
1:A:1080:ASP:O	1:A:1084:ASN:N	2.42	0.49
1:B:770:ILE:HD12	1:B:780:GLN:HE22	1.77	0.49



	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:893:MET:H	1:B:893:MET:CE	2.22	0.49
1:B:1394:ASP:O	1:B:1395:ILE:HD12	2.12	0.49
1:B:422:GLU:N	1:B:422:GLU:OE1	2.45	0.49
1:B:746:ILE:HD13	1:B:760:LEU:HD22	1.94	0.49
1:B:2530:ARG:NH1	1:B:2530:ARG:HB2	2.28	0.49
1:B:2728:ASP:HA	1:B:2731:TYR:HB3	1.94	0.49
1:A:2243:GLU:O	1:A:2258:GLN:NE2	2.45	0.49
1:A:359:ASP:OD1	1:A:360:LEU:N	2.46	0.49
1:A:2530:ARG:HD3	1:A:2656:LYS:HE2	1.95	0.49
1:A:798:ASN:O	1:A:813:ARG:NE	2.38	0.49
1:A:1406:VAL:HG23	1:A:1817:VAL:HG12	1.95	0.49
1:B:1392:THR:O	1:B:1459:LYS:NZ	2.44	0.48
1:A:367:ASP:OD1	1:A:367:ASP:N	2.34	0.48
1:A:1178:THR:HA	1:A:1242:THR:O	2.13	0.48
1:B:68:CYS:SG	1:B:69:ARG:N	2.87	0.48
1:A:463:GLN:HB2	1:A:465:TYR:HE1	1.76	0.48
1:A:886:GLU:HB2	1:A:889:ARG:HH21	1.78	0.48
1:A:890:GLN:HA	1:A:893:MET:SD	2.54	0.48
1:A:2576:TYR:O	1:A:2580:ARG:N	2.46	0.48
1:A:390:LEU:HD23	1:A:411:HIS:CG	2.48	0.48
1:A:1124:ARG:NH2	1:A:1177:ASP:O	2.44	0.48
1:B:878:GLN:HE22	1:B:882:ARG:CZ	2.26	0.48
1:B:2529:PHE:O	1:B:2532:ILE:HG22	2.14	0.48
1:A:2238:ARG:NH2	1:A:2274:VAL:HG12	2.28	0.48
1:A:2647:ALA:C	1:A:2650:PRO:HD2	2.34	0.48
1:B:47:THR:N	1:B:63:GLU:OE1	2.46	0.48
1:B:1248:LYS:HA	1:B:1248:LYS:HE3	1.94	0.48
1:A:893:MET:HA	1:A:896:GLU:HB3	1.95	0.48
1:B:2504:LEU:HD23	1:B:2517:ARG:HH22	1.79	0.47
1:A:2311:ASN:OD1	1:A:2311:ASN:N	2.47	0.47
1:A:2746:PHE:CG	1:A:2750:PRO:HD3	2.49	0.47
1:B:426:LEU:HD23	1:B:437:ALA:HB3	1.95	0.47
1:B:1522:ARG:HA	1:A:1864:ASP:HB3	1.95	0.47
1:A:794:GLN:NE2	1:A:816:ASN:OD1	2.47	0.47
1:A:873:LYS:HA	1:A:873:LYS:HE2	1.95	0.47
1:A:494:TRP:HE3	1:A:495:GLY:H	1.63	0.47
1:B:2266:ARG:NH1	1:B:2271:PRO:O	2.47	0.47
1:A:1395:ILE:HG12	1:A:1395:ILE:O	2.15	0.47
1:A:1847:ASP:OD2	1:A:2188:ARG:NH2	2.48	0.47
1:A:2519:GLY:HA3	1:A:2525:ARG:NH1	2.29	0.47
1:B:2224:LYS:HD3	1:B:2225:PHE:N	2.30	0.47



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2507:GLN:HB3	1:B:2511:ARG:NH2	2.26	0.47
1:A:38:PRO:N	1:A:39:PRO:HD2	2.29	0.47
1:A:936:LYS:O	1:A:936:LYS:HD3	2.14	0.47
1:B:2207:GLU:O	1:B:2210:SER:OG	2.30	0.47
1:B:737:LYS:O	1:B:776:GLY:HA2	2.15	0.47
1:A:463:GLN:HB2	1:A:465:TYR:CE1	2.50	0.47
1:A:1195:GLU:HB3	1:A:1224:LYS:HZ2	1.80	0.47
1:A:2602:PHE:CD2	1:A:2618:ILE:HG12	2.50	0.47
1:A:2729:LEU:HD13	1:A:2791:ILE:HD11	1.96	0.47
1:A:2186:LEU:HD21	1:A:2215:LEU:HD21	1.96	0.46
1:A:2240:LEU:HD13	1:A:2241:SER:N	2.29	0.46
1:A:2276:ARG:HB2	1:A:2276:ARG:CZ	2.44	0.46
1:B:1205:LEU:HD13	1:B:1237:LYS:HD2	1.97	0.46
1:A:846:MET:HG3	1:A:867:ILE:HG12	1.97	0.46
1:B:876:LEU:HD22	1:B:891:TYR:CD1	2.50	0.46
1:B:912:ILE:HG13	1:B:1105:LEU:HD13	1.97	0.46
1:B:1961:MET:HG3	1:B:2171:PRO:CB	2.39	0.46
1:A:425:VAL:HG23	1:A:426:LEU:HG	1.97	0.46
1:A:2529:PHE:CD2	1:A:2650:PRO:HB3	2.51	0.46
1:B:67:VAL:HG21	1:B:374:ILE:HD11	1.96	0.46
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.84	0.46
1:B:2195:LEU:O	1:B:2199:VAL:HG23	2.15	0.46
1:A:11:LEU:HD23	1:A:863:LYS:HB3	1.98	0.46
1:B:1216:HIS:CD2	1:B:1219:HIS:ND1	2.65	0.46
1:B:1345:PHE:O	1:B:1427:ARG:NH2	2.48	0.46
1:B:2512:GLY:O	1:B:2549:THR:OG1	2.29	0.46
1:B:469:GLN:O	1:B:472:ARG:NH2	2.46	0.46
1:B:1197:ARG:HG2	1:B:1197:ARG:HH11	1.81	0.46
1:A:499:PHE:O	1:A:503:LYS:N	2.37	0.46
1:A:1213:ARG:HG3	1:A:1213:ARG:NH1	2.31	0.46
1:A:2519:GLY:HA3	1:A:2525:ARG:HH11	1.81	0.46
1:B:1951:PHE:CE2	1:B:2193:LEU:HD21	2.51	0.45
1:B:2107:ASN:O	1:B:2111:VAL:HG23	2.16	0.45
1:A:2234:ASN:OD1	1:A:2235:GLN:N	2.48	0.45
1:A:2602:PHE:HD1	1:A:2626:VAL:HG22	1.81	0.45
1:B:1182:THR:HB	1:B:1319:LEU:HB2	1.98	0.45
1:B:1318:ASP:OD1	1:B:1318:ASP:N	2.33	0.45
1:B:2244:VAL:HA	1:B:2254:GLN:CD	2.37	0.45
1:B:2239:ASP:OD1	1:B:2240:LEU:N	2.49	0.45
1:A:733:ARG:O	1:A:735:PRO:HD3	2.16	0.45
1:A:1197:ARG:HH21	1:A:1202:LEU:HD11	1.80	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1803:PRO:HB2	1:A:1804:LYS:HD2	1.97	0.45
1:B:390:LEU:H	1:B:390:LEU:HD23	1.80	0.45
1:B:1320:GLU:OE1	1:B:1320:GLU:HA	2.16	0.45
1:A:908:LEU:H	1:A:908:LEU:HD23	1.82	0.45
1:B:766:VAL:HG23	1:B:788:SER:HB2	1.98	0.45
1:B:876:LEU:HD12	1:B:879:HIS:HB2	1.99	0.45
1:B:1266:THR:HG23	1:B:1341:SER:HB2	1.99	0.45
1:B:2525:ARG:HG3	1:B:2525:ARG:NH1	2.31	0.45
1:A:476:LEU:HD23	1:A:485:ALA:HA	1.99	0.45
1:A:882:ARG:HH12	1:A:884:ASP:CG	2.18	0.45
1:A:2583:ILE:HD11	1:A:2635:VAL:HG21	1.98	0.45
1:B:770:ILE:HD12	1:B:780:GLN:NE2	2.31	0.45
1:B:2510:LYS:HB2	1:B:2513:PHE:CD2	2.52	0.45
1:B:2721:MET:HG3	1:B:2725:GLU:OE1	2.16	0.45
1:A:893:MET:H	1:A:893:MET:CE	2.29	0.45
1:A:1112:ARG:HG3	1:A:1114:MET:HG3	1.99	0.45
1:A:1348:GLN:O	1:A:1349:GLU:HB3	2.17	0.45
1:A:2182:HIS:CG	1:A:2183:ASP:H	2.35	0.45
1:B:1137:GLN:HG2	1:B:1154:PHE:CE1	2.52	0.45
1:B:2678:LEU:HD12	1:B:2678:LEU:HA	1.78	0.45
1:B:2723:MET:SD	1:B:2723:MET:N	2.89	0.45
1:A:19:ASN:O	1:A:23:ARG:HG3	2.17	0.45
1:A:892:LEU:HD23	1:A:892:LEU:HA	1.73	0.45
1:A:2759:ASP:OD1	1:A:2759:ASP:N	2.50	0.45
1:B:2308:LYS:NZ	1:B:2501:ASN:OD1	2.34	0.45
1:B:2505:PHE:HD2	1:B:2514:TYR:HD2	1.63	0.45
1:B:2562:LYS:HD3	1:B:2562:LYS:C	2.37	0.45
1:A:55:PRO:HD2	1:A:395:TRP:CZ2	2.51	0.45
1:A:2542:GLN:HB2	1:A:2544:GLU:OE1	2.17	0.44
1:A:821:PRO:HG2	1:A:833:PRO:HB3	2.00	0.44
1:A:479:CYS:HB3	1:A:751:VAL:HG22	2.00	0.44
1:A:2224:LYS:NZ	1:A:2224:LYS:HB3	2.32	0.44
1:B:25:VAL:HG23	1:B:838:LEU:HD21	2.00	0.44
1:B:2258:GLN:HA	1:B:2261:ASN:HD21	1.83	0.44
1:B:2680:ASN:N	1:B:2680:ASN:OD1	2.50	0.44
1:B:2296:TYR:HA	1:B:2299:ILE:HG22	2.00	0.44
1:A:804:ALA:HB3	1:A:808:SER:HB3	1.99	0.44
1:A:2259:LEU:HB2	1:A:2531:ASN:HD21	1.83	0.44
1:B:736:LYS:HG3	1:B:737:LYS:HG2	1.99	0.44
1:A:380:GLU:OE2	1:A:392:GLN:HA	2.17	0.44
1:A:394:LYS:HB3	1:A:397:GLU:OE1	2.16	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2182:HIS:CD2	1:B:2182:HIS:H	2.35	0.44
1:B:2513:PHE:HB3	1:B:2551:ASN:HB3	2.00	0.44
1:B:2721:MET:HG2	1:B:2726:ARG:NH1	2.33	0.44
1:A:37:HIS:ND1	1:A:38:PRO:HD2	2.33	0.44
1:A:915:ARG:HD2	1:A:919:ASN:OD1	2.17	0.44
1:A:2297:THR:O	1:A:2301:GLN:HG2	2.18	0.44
1:B:759:VAL:HG12	1:B:801:ILE:HD11	2.00	0.44
1:A:1138:LYS:O	1:A:1141:LYS:NZ	2.51	0.44
1:B:1098:LEU:O	1:B:1099:GLN:C	2.56	0.43
1:A:2189:TRP:O	1:A:2193:LEU:HG	2.18	0.43
1:A:2733:TRP:HB3	1:A:2734:THR:HG23	1.99	0.43
1:B:430:ASN:HB2	1:B:478:CYS:SG	2.57	0.43
1:B:1841:TRP:HZ3	1:B:1950:VAL:HG11	1.82	0.43
1:B:2526:LEU:HD13	1:B:2649:GLN:NE2	2.32	0.43
1:B:2714:PHE:O	1:B:2718:VAL:HG23	2.18	0.43
1:B:2211:ILE:HA	1:B:2214:GLU:OE1	2.18	0.43
1:A:1381:ASP:OD1	1:A:1431:SER:OG	2.34	0.43
1:A:1444:ALA:HB2	1:A:1499:LEU:HB3	2.00	0.43
1:A:2709:GLN:N	1:A:2709:GLN:NE2	2.53	0.43
1:B:1147:SER:O	1:B:1147:SER:OG	2.33	0.43
1:A:862:LYS:HD2	1:A:863:LYS:HG3	2.01	0.43
1:A:1179:CYS:SG	1:A:1180:SER:N	2.92	0.43
1:A:1940:ASP:O	1:A:1943:SER:OG	2.35	0.43
1:B:385:SER:OG	1:B:386:SER:N	2.52	0.43
1:B:505:MET:HA	1:B:508:LYS:HE2	2.01	0.43
1:B:1203:GLU:CD	1:B:1204:SER:H	2.22	0.43
1:A:2664:LYS:HA	1:A:2664:LYS:HE3	2.00	0.43
1:B:38:PRO:N	1:B:39:PRO:HD2	2.34	0.43
1:B:1965:THR:HG22	1:B:2171:PRO:O	2.19	0.43
1:B:905:LEU:HB3	1:B:907:MET:SD	2.59	0.42
1:A:452:SER:HA	1:A:455:ALA:HB3	2.01	0.42
1:A:1186:ALA:N	1:A:1187:GLU:OE1	2.52	0.42
1:A:2534:ARG:HD2	1:A:2657:GLY:HA2	2.00	0.42
1:B:504:LYS:HA	1:B:507:GLU:OE2	2.20	0.42
1:B:2788:LEU:HA	1:B:2791:ILE:HB	2.01	0.42
1:A:464:THR:OG1	1:A:469:GLN:NE2	2.48	0.42
1:A:851:LEU:H	1:A:851:LEU:HD12	1.84	0.42
1:A:16:ASP:OD1	1:A:16:ASP:N	2.51	0.42
1:B:379:SER:HB2	1:B:380:GLU:OE1	2.19	0.42
1:B:2252:ILE:HD12	1:B:2303:PHE:CE1	2.54	0.42
1:A:2240:LEU:HB3	1:A:2277:VAL:HG22	2.01	0.42



	in a second	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:370:LYS:O	1:B:386:SER:OG	2.37	0.42
1:B:1442:GLU:HG3	1:A:1914:ARG:HD3	2.00	0.42
1:A:18:LEU:O	1:A:22:LEU:HG	2.20	0.42
1:B:1349:GLU:HB3	1:B:1355:SER:CB	2.49	0.42
1:A:24:GLU:H	1:A:24:GLU:CD	2.22	0.42
1:A:421:ASN:OD1	1:A:421:ASN:N	2.44	0.42
1:A:2630:ASN:O	1:A:2634:TYR:N	2.45	0.42
1:B:2731:TYR:CD1	1:B:2735:SER:HA	2.51	0.42
1:A:377:LEU:HD23	1:A:382:LEU:HG	2.01	0.42
1:A:389:GLU:OE1	1:A:389:GLU:N	2.53	0.42
1:A:1809:VAL:HG13	1:A:1813:ILE:HD12	2.00	0.42
1:A:2763:PRO:HG3	1:A:2774:VAL:HG13	2.02	0.42
1:B:70:ILE:HD12	1:B:70:ILE:HA	1.87	0.42
1:B:862:LYS:HA	1:B:862:LYS:HE2	2.01	0.42
1:A:387:LYS:HE2	1:A:387:LYS:N	2.25	0.42
1:A:862:LYS:HD2	1:A:862:LYS:C	2.40	0.42
1:B:499:PHE:HB3	1:B:500:SER:H	1.63	0.42
1:B:741:PRO:HG2	1:B:767:ARG:HH21	1.85	0.42
1:B:939:LYS:H	1:B:939:LYS:HD3	1.85	0.42
1:A:1331:ARG:HG3	1:A:1331:ARG:HH11	1.84	0.42
1:B:68:CYS:SG	1:B:360:LEU:HG	2.60	0.41
1:A:473:ILE:HD13	1:A:487:LEU:HD11	2.03	0.41
1:A:754:LYS:HD2	1:A:754:LYS:C	2.40	0.41
1:A:2035:ILE:CG1	1:A:2037:PRO:HD2	2.50	0.41
1:B:387:LYS:HA	1:B:387:LYS:CE	2.50	0.41
1:B:465:TYR:HB3	1:B:467:GLU:H	1.84	0.41
1:A:1176:ASN:HB3	1:A:1210:GLU:CD	2.40	0.41
1:A:2552:ARG:HG2	1:A:2567:ASP:HB2	2.02	0.41
1:B:1239:LYS:NZ	1:B:1239:LYS:HB3	2.35	0.41
1:A:1823:ASP:N	1:A:1823:ASP:OD1	2.52	0.41
1:A:1873:HIS:CG	1:A:1874:ALA:N	2.89	0.41
1:A:2709:GLN:HA	1:A:2712:ARG:HG3	2.02	0.41
1:B:1859:LEU:HD23	1:B:1936:LEU:HD13	2.02	0.41
1:A:1331:ARG:NH1	1:A:1331:ARG:HG3	2.34	0.41
1:A:1959:LYS:HA	1:A:1959:LYS:HD2	1.82	0.41
1:A:2057:LEU:HD12	1:A:2057:LEU:HA	1.57	0.41
1:A:2640:GLU:OE2	1:A:2640:GLU:N	2.53	0.41
1:B:2534:ARG:H	1:B:2534:ARG:HG2	1.59	0.41
1:A:413:ARG:HB3	1:A:417:LEU:HD23	2.03	0.41
1:B:1284:ALA:O	1:B:1287:THR:HG22	2.20	0.41
1:B:2532:ILE:O	1:B:2536:LEU:HG	2.20	0.41



	t i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:68:CYS:SG	1:A:360:LEU:HD21	2.60	0.41
1:A:465:TYR:O	1:A:469:GLN:NE2	2.53	0.41
1:A:2602:PHE:CD1	1:A:2626:VAL:HG22	2.56	0.41
1:B:432:ILE:HD11	1:B:480:ALA:O	2.21	0.41
1:B:877:MET:SD	1:B:916:CYS:HB2	2.61	0.41
1:B:2226:ARG:HB3	1:B:2227:ARG:HH12	1.84	0.41
1:A:2731:TYR:HD1	1:A:2735:SER:HA	1.86	0.41
1:B:754:LYS:NZ	1:B:770:ILE:HD13	2.36	0.41
1:B:760:LEU:HB2	1:B:767:ARG:CZ	2.51	0.41
1:B:876:LEU:HD23	1:B:911:PHE:HE1	1.84	0.41
1:B:904:ASN:OD1	1:B:904:ASN:N	2.54	0.41
1:B:1143:GLU:O	1:B:1145:SER:N	2.53	0.41
1:A:39:PRO:HG2	1:A:40:LEU:HD22	2.03	0.41
1:A:1274:HIS:HB3	1:A:1342:MET:CE	2.50	0.41
1:A:1343:ILE:HA	1:A:1380:LEU:HD13	2.02	0.41
1:B:480:ALA:HB2	1:B:806:GLN:NE2	2.36	0.41
1:B:1197:ARG:HG2	1:B:1197:ARG:NH1	2.36	0.41
1:B:1834:LYS:HZ3	1:B:1834:LYS:HG3	1.68	0.41
1:B:2057:LEU:HD12	1:B:2057:LEU:HA	1.87	0.41
1:B:2557:VAL:HG21	1:B:2651:LEU:HD13	2.02	0.41
1:A:459:GLU:OE1	1:A:459:GLU:HA	2.21	0.41
1:A:802:PHE:CD2	1:A:844:LEU:HD23	2.56	0.41
1:A:876:LEU:HD23	1:A:911:PHE:CE1	2.56	0.41
1:A:920:ARG:HG2	1:A:924:HIS:HB3	2.02	0.41
1:A:2297:THR:HG21	1:A:2736:SER:HA	2.03	0.41
1:A:2540:LEU:HD23	1:A:2540:LEU:HA	1.86	0.41
1:A:2723:MET:HA	1:A:2726:ARG:HG3	2.03	0.41
1:B:504:LYS:HG3	1:B:508:LYS:HZ3	1.86	0.41
1:B:1179:CYS:SG	1:B:1180:SER:N	2.94	0.41
1:B:2252:ILE:O	1:B:2256:MET:HB2	2.21	0.41
1:B:2293:ARG:NH2	1:B:2767:THR:O	2.54	0.41
1:A:886:GLU:O	1:A:889:ARG:HB3	2.21	0.41
1:A:2617:LEU:HD23	1:A:2641:HIS:CD2	2.49	0.41
1:B:2229:MET:HE1	1:B:2662:LEU:HD22	2.04	0.40
1:B:2541:LEU:HB3	1:B:2542:GLN:OE1	2.20	0.40
1:A:1239:LYS:H	1:A:1239:LYS:HG2	1.77	0.40
1:A:1409:LEU:O	1:A:1418:ARG:NE	2.54	0.40
1:A:1867:HIS:HD2	1:A:1868:PRO:HD2	1.84	0.40
1:B:11:LEU:HD23	1:B:12:PRO:HA	2.02	0.40
1:B:893:MET:HE3	1:B:893:MET:N	2.30	0.40
1:B:1438:ILE:HG23	1:A:1918:LEU:HD13	2.03	0.40



Continueu from previous page					
Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:1493:PRO:O	1:B:1780:SER:HB3	2.21	0.40		
1:B:2212:LEU:HD23	1:B:2212:LEU:HA	1.88	0.40		
1:B:2522:THR:O	1:B:2526:LEU:HG	2.21	0.40		
1:B:2556:LYS:HG2	1:B:2561:ARG:HB3	2.02	0.40		
1:A:1195:GLU:OE1	1:A:1197:ARG:HD2	2.21	0.40		
1:A:2240:LEU:O	1:A:2277:VAL:HA	2.22	0.40		
1:A:2766:ASN:O	1:A:2770:SER:N	2.55	0.40		
1:B:745:GLU:OE1	1:B:747:LEU:HD22	2.21	0.40		
1:B:2099:PRO:O	1:A:1370:TYR:OH	2.21	0.40		
1:A:880:ILE:HD12	1:A:880:ILE:N	2.36	0.40		
1:A:882:ARG:O	1:A:1081:ARG:NH1	2.55	0.40		
1:A:1468:LEU:HD22	1:A:1802:ILE:HD11	2.04	0.40		
1:B:457:LYS:HD2	1:B:457:LYS:HA	1.91	0.40		
1:A:2034:CYS:O	1:A:2036:PRO:HD3	2.21	0.40		
1:A:2262:HIS:CE1	1:A:2266:ARG:HE	2.39	0.40		
1:B:417:LEU:HD12	1:B:460:HIS:O	2.22	0.40		
1:B:1962:ASN:ND2	1:B:2181:SER:HA	2.37	0.40		
1:B:2753:THR:N	1:B:2772:LEU:O	2.45	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	ntile	\mathbf{s}
1	А	1533/2830~(54%)	1456 (95%)	75 (5%)	2(0%)	51	85	
1	В	1604/2830~(57%)	1506 (94%)	93~(6%)	5(0%)	41	76	
All	All	3137/5660~(55%)	2962 (94%)	168 (5%)	7 (0%)	50	82	

All (7) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	462	ALA
1	В	499	PHE
1	В	873	LYS
1	А	41	ASN
1	А	2204	VAL
1	В	2178	MET
1	В	1395	ILE

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	Percentiles
1	А	1366/2439~(56%)	1258~(92%)	108 (8%)	12 41
1	В	1438/2439~(59%)	1316~(92%)	122 (8%)	10 38
All	All	2804/4878~(58%)	2574 (92%)	230 (8%)	15 39

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	1	MET
1	В	16	ASP
1	В	18	LEU
1	В	20	ASP
1	В	64	ASP
1	В	377	LEU
1	В	386	SER
1	В	415	THR
1	В	423	LYS
1	В	449	GLU
1	В	451	LEU
1	В	452	SER
1	В	459	GLU
1	В	460	HIS
1	В	478	CYS
1	В	479	CYS
1	В	482	TYR



Mol	Chain	Res	Type
1	В	493	TRP
1	В	499	PHE
1	В	500	SER
1	В	505	MET
1	В	508	LYS
1	В	562	MET
1	В	566	TRP
1	В	568	MET
1	В	572	CYS
1	В	575	GLN
1	В	652	SER
1	В	653	LEU
1	В	733	ARG
1	В	754	LYS
1	В	759	VAL
1	В	761	LYS
1	В	769	CYS
1	В	777	LYS
1	В	803	THR
1	В	807	GLU
1	В	822	MET
1	В	827	MET
1	В	832	ASP
1	В	836	LEU
1	В	849	HIS
1	В	873	LYS
1	В	889	ARG
1	В	893	MET
1	В	905	LEU
1	В	907	MET
1	В	914	HIS
1	В	936	LYS
1	В	938	THR
1	В	939	LYS
1	В	1077	GLU
1	В	1084	ASN
1	В	1094	ASP
1	В	1112	ARG
1	В	1138	LYS
1	В	1141	LYS
1	B	1147	SER
1	В	1177	ASP



Mol	Chain	Res	Type
1	В	1179	CYS
1	В	1195	GLU
1	В	1237	LYS
1	В	1239	LYS
1	В	1240	CYS
1	В	1271	ARG
1	В	1280	VAL
1	В	1290	HIS
1	В	1291	CYS
1	В	1317	HIS
1	В	1323	ARG
1	В	1341	SER
1	В	1344	MET
1	В	1354	LEU
1	В	1355	SER
1	В	1362	HIS
1	В	1382	CYS
1	В	1392	THR
1	В	1404	THR
1	В	1413	TYR
1	В	1507	MET
1	В	1508	GLN
1	В	1511	GLU
1	В	1522	ARG
1	В	1804	LYS
1	В	1810	TYR
1	В	1838	THR
1	В	1861	SER
1	В	2114	MET
1	В	2115	GLN
1	В	2167	THR
1	В	2172	GLN
1	В	2174	SER
1	В	2182	HIS
1	В	2184	MET
1	В	2198	ARG
1	В	2201	MET
1	В	2218	PHE
1	В	2222	GLU
1	В	2224	LYS
1	В	2251	LEU
1	В	2272	MET



Mol	Chain	Res	Type
1	В	2294	SER
1	В	2501	ASN
1	В	2511	ARG
1	В	2517	ARG
1	В	2525	ARG
1	В	2529	PHE
1	В	2553	HIS
1	В	2568	PHE
1	В	2571	PHE
1	В	2586	SER
1	В	2598	MET
1	В	2635	VAL
1	В	2649	GLN
1	В	2655	ARG
1	В	2689	MET
1	В	2714	PHE
1	В	2721	MET
1	В	2728	ASP
1	В	2733	TRP
1	В	2749	MET
1	В	2762	LEU
1	А	1	MET
1	А	2	THR
1	А	16	ASP
1	А	37	HIS
1	А	387	LYS
1	А	395	TRP
1	А	457	LYS
1	А	464	THR
1	А	465	TYR
1	А	479	CYS
1	А	491	LEU
1	А	494	TRP
1	А	505	MET
1	А	550	SER
1	A	552	SER
1	А	562	MET
1	A	563	GLU
1	A	572	CYS
1	A	573	ARG
1	A	576	LEU
1	А	651	TRP



Mol	Chain	Res	Type
1	А	653	LEU
1	А	681	LYS
1	А	737	LYS
1	А	754	LYS
1	А	787	SER
1	А	788	SER
1	А	803	THR
1	А	806	GLN
1	А	818	THR
1	А	836	LEU
1	А	838	LEU
1	А	862	LYS
1	А	882	ARG
1	А	893	MET
1	А	907	MET
1	А	911	PHE
1	А	913	SER
1	А	1094	ASP
1	А	1112	ARG
1	A	1114	MET
1	A	1139	ILE
1	А	1151	GLU
1	A	1157	MET
1	A	1161	SER
1	A	1179	CYS
1	A	1189	ILE
1	A	1192	ASP
1	A	1195	GLU
1	A	1197	ARG
1	A	1248	LYS
1	A	1291	CYS
1	A	1335	ASP
1	A	1341	SER
1	A	1355	SER
1	A	1411	ASN
1	A	1412	LYS
1	A	1431	SER
1	A	1455	GLN
1	A	1499	LEU
1	A	1507	MET
1	A	1776	SER
1	A	1779	THR



Mol	Chain	Res	Type
1	А	1807	HIS
1	А	1820	THR
1	А	1823	ASP
1	А	1861	SER
1	А	1929	ASN
1	А	2063	LYS
1	А	2184	MET
1	А	2194	GLU
1	А	2198	ARG
1	А	2215	LEU
1	А	2221	LYS
1	А	2222	GLU
1	А	2227	ARG
1	A	2229	MET
1	A	2231	LYS
1	А	2238	ARG
1	А	2239	ASP
1	А	2246	ARG
1	А	2248	ARG
1	А	2275	HIS
1	А	2280	THR
1	А	2284	GLU
1	А	2309	LEU
1	А	2504	LEU
1	А	2523	GLU
1	А	2534	ARG
1	А	2543	ASN
1	А	2553	HIS
1	А	2565	TRP
1	А	2595	PHE
1	А	2600	LEU
1	А	2632	TYR
1	A	2636	ARG
1	A	2655	ARG
1	A	2656	LYS
1	A	2664	LYS
1	A	2673	GLU
1	А	2709	GLN
1	A	2721	MET
1	А	2723	MET
1	A	2725	GLU
1	А	2738	SER



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Mol	Chain	Res	Type
1	А	2742	SER
1	А	2759	ASP
1	А	2777	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	405	GLN
1	В	411	HIS
1	В	430	ASN
1	В	890	GLN
1	А	1870	HIS
1	А	1962	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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-16087. 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: 150



Y Index: 150



Z Index: 150

6.2.2 Raw map



X Index: 150

Y Index: 150

Z Index: 150

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: 135



Y Index: 172



Z Index: 107

6.3.2 Raw map



X Index: 137

Y Index: 150



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 0.0632. 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.

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 180 nm^3 ; this corresponds to an approximate mass of 162 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 0.333 ${\rm \AA^{-1}}$



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 0.333 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	-	3.00	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	8.20	4.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 8.20 differs from the reported value 3.0 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16087 and PDB model 8BJA. 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 0.0632 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 (0.0632).



9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0632) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.3630
А	0.7500	0.3700
В	0.7200	0.3570



