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PDB ID	:	8WYD
EMDB ID	:	EMD-37924
Title	:	Cryo-EM structure of DSR2-DSAD1 complex
Authors	:	Zhang, J.T.; Jia, N.; Liu, X.Y.
Deposited on	:	2023-10-30
Resolution	:	2.56 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:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.56 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.



wietric	$(\# { m Entries})$	$(\# { m Entries})$
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	of chain		
1	А	1005	6 7%		27%	• 5%
1	В	1005	6 8%		25%	• 5%
1	С	1005	66% 66%		27%	• 5%
1	D	1005	65% 66%		27%	• 5%
2	Е	146	46%	28%	5%	21%
2	F	146	79% 51%	27%	·	21%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 33765 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.

Mol	Chain	Residues		А		AltConf	Trace		
1	Δ	053	Total	С	Ν	Ο	S	0	0
1	Π	900	7964	5163	1285	1484	32	0	0
1	В	052	Total	С	Ν	Ο	\mathbf{S}	0	0
1	D	900	7966	5162	1288	1486	30	0	0
1	C	052	Total	С	Ν	Ο	S	0	0
1	U	932	7955	5157	1283	1483	32	0	0
1	Л	052	Total	С	Ν	Ο	S	0	0
1	D	900	7966	5162	1288	1486	30	0	0

• Molecule 1 is a protein called SIR2 family protein.

• Molecule 2 is a protein called Bacillus phage SPbeta DSAD1 protein.

Mol	Chain	Residues		At	oms	AltConf	Trace			
2	F	116	Total	С	Ν	Ο	S	0	0	
2	Ľ	110	957	625	154	175	3	0	0	
0	Б	116	Total	С	Ν	0	S	0	0	
2	Ľ	110	957	625	154	175	3		0	

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	121	TRP	-	expression tag	UNP O64191
Е	122	SER	-	expression tag	UNP O64191
E	123	HIS	-	expression tag	UNP O64191
E	124	PRO	-	expression tag	UNP O64191
E	125	GLN	-	expression tag	UNP O64191
E	126	PHE	-	expression tag	UNP O64191
E	127	GLU	-	expression tag	UNP O64191
E	128	LYS	-	expression tag	UNP O64191
E	129	GLY	-	expression tag	UNP O64191
Е	130	GLY	-	expression tag	UNP O64191
E	131	GLY	-	expression tag	UNP O64191
Е	132	SER	-	expression tag	UNP O64191
Е	133	GLY	-	expression tag	UNP O64191



Continu	led from pre	vious page			
Chain	Residue	Modelled	Actual	Comment	Reference
E	134	GLY	-	expression tag	UNP 064191
E	135	GLY	-	expression tag	UNP 064191
E	136	SER	-	expression tag	UNP 064191
E	137	GLY	-	expression tag	UNP 064191
E	138	GLY	-	expression tag	UNP 064191
E	139	TRP	-	expression tag	UNP 064191
Ε	140	SER	-	expression tag	UNP 064191
Ε	141	HIS	-	expression tag	UNP 064191
E	142	PRO	-	expression tag	UNP 064191
Е	143	GLN	-	expression tag	UNP 064191
Е	144	PHE	-	expression tag	UNP 064191
Е	145	GLU	-	expression tag	UNP 064191
Е	146	LYS	-	expression tag	UNP 064191
F	121	TRP	-	expression tag	UNP 064191
F	122	SER	-	expression tag	UNP 064191
F	123	HIS	-	expression tag	UNP 064191
F	124	PRO	-	expression tag	UNP 064191
F	125	GLN	-	expression tag	UNP 064191
F	126	PHE	-	expression tag	UNP 064191
F	127	GLU	-	expression tag	UNP 064191
F	128	LYS	-	expression tag	UNP 064191
F	129	GLY	-	expression tag	UNP 064191
F	130	GLY	-	expression tag	UNP 064191
F	131	GLY	-	expression tag	UNP 064191
F	132	SER	-	expression tag	UNP 064191
F	133	GLY	-	expression tag	UNP 064191
F	134	GLY	-	expression tag	UNP 064191
F	135	GLY	-	expression tag	UNP 064191
F	136	SER	-	expression tag	UNP 064191
F	137	GLY	-	expression tag	UNP 064191
F	138	GLY	-	expression tag	UNP 064191
F	139	TRP	-	expression tag	UNP 064191
F	140	SER	-	expression tag	UNP 064191
F	141	HIS	-	expression tag	UNP 064191
F	142	PRO	-	expression tag	UNP 064191
F	143	GLN	-	expression tag	UNP 064191
F	144	PHE	-	expression tag	UNP 064191
F	145	GLU	-	expression tag	UNP 064191
F	146	LYS	-	expression tag	UNP 064191

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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: SIR2 family protein





• Molecule 1: SIR2 family protein







D1 01 F1 07 F1 07 F1 07 F1 07 F1 17 F1 17 F1 17 D1 35 D1 35 D1 35 D1 35 D1 35 D1 40 D1 40 D1 41 D1 41 D1 41 D1 41 D1 61 D1 610	RI 45 0145 1147 1152 1152 1152 1152 1152 1152 1152 115	L191 N192 N196 L220 L229 N230 R236 R233 R233 R233 R236 R236 R236 R236	
L266 N278 N278 281 281 281 281 281 297 8296 4297 8298 8298 7301 7302	K304 N305 D306 Caracter V308 V308 V308 V308 V308 V308 V308 V313 V313 V314 V315	F320 F321 F321 F325 F325 F325 F325 F328 F332 F334 F331 F335 F335 F335 F335 F335	D337 V338 F340 E341 V342 C344 V345 V346
V347 R348 H349 K360 K361 K361 K362 C363 F364 C365 C365 C365 C365 C365 C365 C365 C365	E361 E362 E362 E365 E365 E365 E365 E365 E365 E365 E365	4377 7378 7378 6379 6381 7382 7383 7384 7383 7384 73855 73855 73855 738555 7385555555555555555555555555555555555	1394 C395 A397 A397 A397 A397 A400 G401 T402 N404 T405 S406
Ido7 Ed08 1d09 8d11 8d11 8d11 8d12 8d12 8d14 8d15 7d18 8d16 8d16 8d16 8d16 8d16 8d18 9d19 9d19	M421 K422 K423 F424 E426 E426 C426 C428 C428 C430 S431 F432 S431 F432 S431 F432 S431 F432 S431 F432 S431 F432 S431 F432 S431 F432 S433 S431 F432 S431 F432 F433 S431 F432 F432 F432 F432 F432 F432 F432 F432	Y436 K437 K438 A439 F440 F441 L442 A443 A443 C444 A443 C445 C444 C445 F445 F445 F445 F445 F445	I454 + Y455 + S456 + M457 + I458 + I459 + S422 + M461 + S422 + S427 +
ASN 6468 4470 4471 4471 4472 6475 6475 6475 6475 8478 8478 8480 4480	Y482 4482 5484 1485 4485 4486 4487 4489 4491 4490 4491 4495 4495 4495 4496 4496 4496 4496	L497 L498 F500 F500 G501 H502 K504 F503 F505 F505 F505 F505 F505 F505 F501 F511 F51	H514 1515 1515 1616 16517 1617 1620 17520 1623 1623 1624
2 8 8 8 8 8 8 8 8 8 8 8 9 4 4 9	1 1 <td>6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6</td> <td>77 777 778 88 88 88 88 88 88 88 88 88 88</td>	6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	77 777 778 88 88 88 88 88 88 88 88 88 88
			SHR SHR SHR SHR CLYS CLYS CLYS CLYS SC40 641 7641 641
E648 Y650 Y650 P651 F652 V653 N654 R657 H657 H658 F650 K660	D662 D663 1664 K665 K665 L667 E667 E668 S670 S670 1673 1673	R677 F678 6679 6679 6680 1684 1684 1684 1688 1694 1691 1691 1691	1696 7697 6698 7699 7699 7700 7703 7700 7703 7705 7705 7705
F708 Y709 T710 7711 7712 7712 7713 5714 5715 7716 7716 7716 7718 7718 7718 7718	F722 A723 K724 Y726 Y726 V726 K727 E731 E730 E731 C732 E731 C732 E731 C733 C734 C735 T736	V737 V739 A739 L740 L741 F743 F744 F745 F745 F745 F745 F745 F745 F745	Y755 V756 W757 L758 E759 E750 L761 T762 C764 N765 C764 L767 L767
P768 K769 S770 S770 1771 1772 S773 S773 1774 D776 D776 F778 D777 F778 L778 V780 V780	q782 A783 E784 H785 H785 Q789 Q789 Q789 Q789 N791 S792 S792 S795 S795 S795	N797 0798 1799 1799 17800 1800 1802 1807 1807 1808 1811	F815 1816 8817 8817 8818 8821 1820 8821 1822 1823 1823 1825 1825 1825 1825 1825 1825 1827
T828 Q829 Q820 Q830 Q831 Q832 Q834 Q835 Q834 Q840 Q840 Q840 Q840 Q840	L842 P843 L844 L844 L845 S846 R849 A849 A849 A849 A848 A849 A848 A848 A	K857 S858 S858 S858 S858 B860 B861 B861 B861 B863 B863 B865 B865 B865 B865 B865 B865 B865 B865	B875 E876 F877 F877 P879 P881 L884 L885 L885 L885 E887
Y888 L889 E890 F891 K893 V894 V894 V895 V895 C1U VAL C1V C1V C1V C1V C1V	ILE CLY CLN CLN CLN CLN CLE CLE SER SSER SSER SSER SSER SSER SSER SSE	Y920 F921 L922 E923 E924 N925 N926 N926 N926 E931 E931 F933 F933 F933 F933 F935 F935 F936 H9836	D938 Y940 Y940 F942 F943 Y946 P945 P945 P945
948 948 950 951 955 955 955 955 955 956 950 950 950 950 950	962 963 964 965 965 965 965 971 971 975 975 975	1977 1976 1980 1980 1980 1980 1980 1990 1991 1991	1005
• Molecule 1: SIR2 famil	ly protein		<u> </u>

65% Chain D: 66% 27% • 5%



MET VAL	LYS VAL	ASP	GLU	83	K9	Y11	G12	E13 K14		K16	E1 (V18	F19	M21	L22	D23	1-7N	C29 130	c F	100	S37 R38	6 VA	V43 F44	F45 V46	G47	Y56	E69	P74	LYS	GLY ASN	Y79 S80	S81	Y84	V9 <mark>4</mark> K95	F107	D116	0111						
K120	A123	M124	N133	Y134 D135	N136	D139	T140	R145 6146	K147	Y148 F149	S150 V151		N160	8163 6164	R165	K169	0 ¹⁷⁰		V183	D188	12 <mark>13</mark>	L220	N230	D022		D249 P250	E256	1259	R267	D270	S273	V 28.7	R 285	0071								
Y286 S287	M290	D291	L292 L293	I 294 E 295	S296	4297 E298	N299	K300 F301	1302	T303	K304 D305	D306	E307	V308	1309 D310	Y311	1312	G314	K315	I316 S317	P318	L319	A321	L322	Q323	1325	R326	1328	D329	K331	H332 V333	F334	F336	D337	H339	F340	E341 V342	N343	G344 T345	V346		
V347	H349	K350	N351	K352 G353	F354	G355	Y356	E358	R359	F360	E362	L363	E365	s366	C367	D368	E309 R370	S371	K372	s374	K375	K376	u3// ¥378 ♦	E379	R380 F381	N382	A383	F385	N386	F388	E389	N391	G392 V393	1394	C395	A397	K398	A400	G401	1403	N404 T405	S406
[407	1409	1410	3411	413	(414	1415	410 (417	(418	0419	421 •	(422	(423	·424 [425	3426	3427	1428	1430	3431	1432	1433 0434	0435	1436	(438	4439	·440	442	1443 2444	445	3446	1448	2449	3451	(452 🔶)453	454	(455 🕈	1457	[459	460	1461 3462	[463	JLU SER	
- <u>-</u>	0 69	1	71	73	74	29 2		70		81	83 83	84 •	85	86	8%		•	10 0 0 0	83 83 83 83	94	95 🔷 I							00 06				12	14 14	15	16 17	18	50 <u>1</u>	21	1 8 1	24 25	50 •	I
	5 S	ν γ		T T	S,		L Ng	3				8 8	5I 0			y V	2 • •	9		55 0 6				PF	RE	H	KE	BC I	<u>ч</u> р			6 0					6 11 12		0 N		DE	
L52	N52	G53	F53		K53	K54	I54	E54	F54		D54	N54	Q54	L55	Y55		T55	V55	K55	F55	E56		N56	K56	ARG		MET	GLY GLU	SER	SER	GLY MET	S57	S58	158	V58	L58	T58	L58	Y58	D59	••	
N591		• F594	L595	Y596	N598	C599		♦	V603	F605	H606	E607	F608		Y611	• I612	R613	• S615	M616	S617	L619	• I620	E621	A623	E624	♥ Y625 ● E626	• R627	T628	D630		E633	L634	F636	PHE	GLY GLY	LYS	SER	G044 F645	F646	E648	Y649	••
D651	r032 V653	N654	I655	S656 R657	H658	F659	K660 T661	D662	D663	I664 K665	N666	L667	E668	S670	C671	S672	I673	K675	1676	R677 F678	G679	E680	ជ្ញ681 FF82	E002 K683	I684	E685 E686	Y687	L688 V689	0690	1691	E693	E694	T696	K697	4030 F699	S700	A701 N702	G7 03	M7 04 N7 05	V7 06 V7 07	F7 08	Y7 09 T7 10
Q711	I7 13	<mark>S714</mark>	E7 15	A716 K717	A718	A7 19	L720 Y721	F722	A723	K7 24 Y7 25	V726	K7 27	L728 6770	51 29 E730	E731	G732	L733 C73A	K735	1736	<mark>V737</mark> V738	A7 39	L740	L741 F743	r 42 Y743	F744	P745 E746	R747	D748 1.749	D750	1751 6750	K753	R754 V755	V756	W757 1760	E7 59	R760	L761 T762	K763	C7 64 N7 65	E766 1767	P768	K769 S770
1771	S773	1774	1775	D777	F778	L779	V780	Q782	A783	E784 K785	H786	1787	D780	062N	Y791	S792	E793 V70A	S795	S796	N797	r199	Y 800	S801	D803	Y804	G 805 A 806	L807		H810	F811	K813	N814 F815	I816	S817	R819	L820	5821 E822	I 823	T824 L825	C826	T828	Q829
K831	4632 K833	Q834	1835	D836 F837	L838	F839	K840 1.841	L842	P843	L844 L845	S846	T847	N848	K850	S851	H852	L853	S855	F856	K857	V859	E860	N861	1002 N863	D864	L865 M866	N867	G868	R870	1871 G870	L873	1874	E876	F877 T070	10/0 P879	E880	H881 E882	E883	L884 1885	I886 F887	Y888	L889 E890
T891	K893	V894	N895	Y 896 T 897	VAL	LYS UL	GLU GLU	GLY	GLN	PHE	SER	ASN	D911	Y912	S914	T915	F916		W919	Y920	r921 L922	E923	E924	1925 N926	N927	8928 K929	M930	E931	F933	1934	926W	D937	1939	Y940	1941 F942	F943	V944 D945	P946	E947 N948	F949	Deer	
Y951	K953	F954	1955	P956	W958	L959	K960	Y962	N963	D964 K965	F966	L967	G968		A971	G972	N973	H975	M976	К977 но78	61979	V980	1981 Бавл	V983	L984	K985 E986	R987	V988	066N	S991	D993	K994 R995	¥996	L997	666I	L1000	M1001 N1002	Y1003	F1004			







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101402	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.225	Depositor
Minimum map value	-2.195	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	463.12003, 463.12003, 463.12003	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	nd lengths	Bo	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.27	0/8148	0.46	0/10973
1	В	0.28	0/8148	0.47	0/10973
1	С	0.28	1/8139~(0.0%)	0.48	5/10962~(0.0%)
1	D	0.27	0/8148	0.46	0/10973
2	Е	0.26	0/983	0.53	1/1333~(0.1%)
2	F	0.26	0/983	0.46	0/1333
All	All	0.27	1/34549~(0.0%)	0.47	6/46547~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	745	PRO	CG-CD	-5.36	1.32	1.50

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	843	PRO	CA-N-CD	-11.87	94.88	111.50
1	С	745	PRO	N-CD-CG	-9.97	88.24	103.20
2	Е	50	PRO	CA-N-CD	-6.07	103.00	111.50
1	С	745	PRO	CA-CB-CG	-5.53	93.50	104.00
1	С	745	PRO	CA-N-CD	-5.29	104.09	111.50
1	С	843	PRO	N-CD-CG	-5.12	95.53	103.20

All (6) bond angle outliers are listed below:

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	7964	0	7812	183	0
1	В	7966	0	7811	181	0
1	С	7955	0	7799	182	0
1	D	7966	0	7811	193	0
2	Е	957	0	942	40	0
2	F	957	0	942	30	0
All	All	33765	0	33117	773	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 12.

All (773) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:52:ARG:HH21	2:E:54:ASN:HA	1.32	0.93
1:C:297:GLN:NE2	1:D:521:ASN:HD21	1.74	0.85
1:C:297:GLN:NE2	1:D:521:ASN:ND2	2.25	0.83
2:F:88:HIS:HD2	2:F:91:THR:H	1.25	0.83
1:C:772:ILE:HD11	1:C:808:ILE:HG23	1.62	0.81
1:D:802:ARG:HB2	1:D:840:LYS:HB3	1.64	0.78
1:D:691:ILE:HD11	1:D:716:ALA:HA	1.66	0.76
1:C:82:ASP:OD1	1:C:82:ASP:N	2.15	0.76
1:A:820:LEU:HD23	1:A:823:ILE:HD11	1.65	0.76
1:A:728:LEU:H	1:A:765:ASN:HD21	1.35	0.75
1:B:122:LEU:HD12	1:B:147:LYS:HD2	1.70	0.74
1:C:505:LYS:NZ	1:C:509:ASP:OD1	2.22	0.73
1:C:709:TYR:OH	1:C:748:ASP:OD2	2.06	0.72
1:C:995:ARG:HE	1:C:999:ILE:HG13	1.54	0.72
1:D:327:LYS:NZ	1:D:391:ASN:O	2.22	0.72
1:B:827:LEU:HD13	1:B:835:ILE:HG22	1.71	0.72
1:C:800:TYR:N	1:C:803:ASP:OD2	2.22	0.71
1:B:776:ASP:HA	1:B:779:LEU:HD12	1.74	0.70
1:A:802:ARG:HH12	1:A:870:ARG:HE	1.39	0.70
1:B:467:ASN:N	1:B:467:ASN:HD22	1.90	0.70
1:A:827:LEU:HD22	1:A:835:ILE:HG12	1.72	0.69
1:B:65:LYS:HD3	1:B:107:PHE:HE2	1.56	0.69
1:B:327:LYS:NZ	1:B:391:ASN:O	2.26	0.69
1:D:366:SER:OG	1:D:369:GLU:OE1	2.11	0.69
1:A:424:PHE:O	1:A:438:LYS:NZ	2.24	0.68
1:A:554:ASP:OD2	1:A:591:ASN:ND2	2.26	0.68
1:D:673:ILE:HD12	1:D:673:ILE:H	1.58	0.68
1:C:777:ASP:OD1	1:C:819:ARG:NH1	2.25	0.68



	to us page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:E:50:PRO:HD3	2:E:61:VAL:HG22	1.75	0.68	
1:C:724:LYS:HE3	1:C:763:LYS:HG3	1.77	0.67	
1:D:315:LYS:NZ	1:D:335:GLU:OE1	2.27	0.67	
2:E:52:ARG:NH2	2:E:54:ASN:HA	2.07	0.66	
1:B:366:SER:OG	1:B:369:GLU:OE1	2.12	0.66	
1:B:841:LEU:HB3	1:B:844:LEU:HD12	1.77	0.66	
1:A:815:PHE:HD2	1:A:844:LEU:HD22	1.59	0.66	
1:D:946:PRO:HB3	1:D:976:MET:HE2	1.77	0.66	
1:C:705:ASN:HB3	1:C:708:PHE:HB3	1.78	0.66	
1:C:446:GLY:HA3	1:C:708:PHE:HB2	1.78	0.66	
1:D:682:GLU:N	1:D:682:GLU:OE1	2.28	0.65	
1:B:37:SER:OG	1:B:124:MET:O	2.14	0.65	
1:C:724:LYS:HB2	1:C:760:ARG:HB3	1.78	0.65	
1:C:741:LEU:HA	1:C:754:ARG:HD3	1.78	0.65	
1:A:801:SER:HA	1:A:804:TYR:HD1	1.61	0.65	
1:D:705:ASN:HB3	1:D:708:PHE:HB3	1.77	0.65	
1:B:919:TRP:HB3	1:B:924:GLU:HB2	1.79	0.64	
1:C:57:PRO:HA	1:C:61:ARG:HH12	1.62	0.64	
1:B:870:ARG:NH2	2:E:75:ILE:O	2.31	0.64	
1:C:480:ARG:NH2	1:C:546:SER:O	2.31	0.64	
1:C:791:TYR:O	1:C:833:LYS:NZ	2.29	0.64	
2:F:88:HIS:CD2	2:F:91:THR:H	2.12	0.64	
1:D:934:ILE:HG23	1:D:941:ASP:HB3	1.79	0.64	
1:A:980:VAL:HG21	1:A:1005:ILE:HG22	1.79	0.64	
1:D:870:ARG:NH2	2:F:75:ILE:O	2.31	0.64	
1:D:912:TYR:HB3	1:D:916:PHE:HE1	1.62	0.64	
1:D:918:ILE:HD13	1:D:966:LEU:HD11	1.79	0.64	
1:C:364:LYS:O	1:C:370:ARG:NH2	2.31	0.64	
1:D:394:ILE:HD12	1:D:395:CYS:H	1.63	0.64	
1:C:19:PHE:HA	1:C:22:LEU:HD12	1.80	0.64	
1:A:483:GLN:O	1:A:487:GLN:HG2	1.97	0.63	
1:D:886:ILE:HD13	1:D:929:LYS:HE2	1.80	0.63	
1:A:489:VAL:HG21	1:A:512:LEU:HD11	1.79	0.63	
1:B:974:LYS:HE2	1:B:974:LYS:HA	1.80	0.63	
1:B:627:ARG:HD2	1:B:675:LYS:HE3	1.79	0.63	
1:C:192:ASN:O	1:C:196:ASN:ND2	2.31	0.63	
2:E:120:ASP:OD1	2:E:121:TRP:N	2.32	0.63	
1:D:433:GLU:N	1:D:433:GLU:OE1	2.31	0.62	
1:D:681:GLN:HG2	1:D:726:VAL:HG23	1.81	0.62	
1:A:771:ILE:O	1:A:775:ILE:HG13	2.00	0.62	
1:D:882:GLU:HB3	1:D:927:ASN:HD22	1.65	0.62	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:668:GLU:OE1	1:A:725:TYR:OH	2.15	0.62
1:D:369:GLU:HA	1:D:372:LYS:HD3	1.82	0.62
1:A:831:LYS:O	1:A:835:ILE:HG13	1.99	0.61
1:D:37:SER:OG	1:D:124:MET:O	2.18	0.61
1:D:561:LEU:HD11	1:D:584:VAL:HG11	1.82	0.61
1:B:984:LEU:HB3	1:B:1000:LEU:HG	1.83	0.61
1:A:476:ILE:HD13	1:A:524:ILE:HD11	1.83	0.61
2:E:67:PHE:HA	2:E:72:ARG:HA	1.82	0.61
1:D:282:TYR:HA	1:D:285:ARG:HE	1.65	0.61
1:D:421:MET:HG3	1:D:445:LEU:HD11	1.83	0.61
1:D:79:TYR:HB3	1:D:84:TYR:HE1	1.65	0.61
1:D:733:LEU:HD22	1:D:765:ASN:HD22	1.65	0.61
1:D:783:ALA:O	1:D:834:GLN:NE2	2.33	0.61
1:B:291:ASP:O	1:B:295:GLU:HG2	2.01	0.60
1:B:476:ILE:HD13	1:B:524:ILE:HD11	1.83	0.60
1:D:724:LYS:HB2	1:D:760:ARG:HB3	1.83	0.60
1:B:148:TYR:O	1:B:165:ARG:NH1	2.35	0.60
1:B:23:ASP:OD1	1:B:24:ASN:N	2.34	0.60
1:C:23:ASP:HB3	1:C:26:VAL:HG23	1.84	0.60
1:C:302:ILE:HD12	1:C:307:GLU:HB3	1.82	0.60
1:C:327:LYS:NZ	1:C:391:ASN:O	2.34	0.60
1:B:835:ILE:HD12	1:B:836:ASP:N	2.16	0.60
1:B:967:LEU:HD22	1:B:1005:ILE:HD13	1.83	0.60
1:A:842:LEU:HD13	1:A:853:LEU:HD23	1.83	0.59
1:D:336:TYR:O	1:D:349:HIS:ND1	2.32	0.59
1:A:477:ASN:O	1:A:481:ILE:HG12	2.02	0.59
1:B:310:ASP:OD1	1:B:380:ARG:NH1	2.36	0.59
1:D:476:ILE:HD13	1:D:524:ILE:HD11	1.84	0.59
1:B:839:PHE:HZ	1:B:873:LEU:HG	1.68	0.59
1:C:721:TYR:O	1:C:760:ARG:NH2	2.35	0.58
1:B:695:ILE:HD11	1:B:744:PHE:HA	1.84	0.58
1:B:832:GLN:NE2	1:B:835:ILE:HD11	2.18	0.58
1:C:476:ILE:HD13	1:C:524:ILE:HD11	1.85	0.58
1:C:836:ASP:HA	1:C:857:LYS:NZ	2.18	0.58
1:D:827:LEU:HD13	1:D:835:ILE:HG13	1.84	0.58
1:A:770:SER:O	1:A:774:ILE:HG12	2.03	0.58
1:A:787:ILE:HD13	1:A:834:GLN:HG3	1.85	0.58
1:D:147:LYS:HE3	1:D:147:LYS:HA	1.86	0.58
1:D:250:PRO:HA	1:D:285:ARG:HH12	1.69	0.58
1:A:238:ASP:OD1	1:A:238:ASP:N	2.37	0.58
1:A:818:LYS:HB2	1:A:819:ARG:NH2	2.19	0.58



	ious page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:226:ASN:OD1	1:C:86:ARG:NH2	2.37	0.58
1:C:310:ASP:OD1	1:C:380:ARG:NH1	2.35	0.58
1:D:758:LEU:HA	1:D:761:LEU:HD12	1.85	0.58
1:A:841:LEU:HD11	1:A:844:LEU:HD12	1.85	0.58
1:C:668:GLU:OE2	1:C:760:ARG:NH1	2.36	0.58
1:A:318:PRO:HB3	1:A:538:LYS:HE3	1.86	0.58
1:C:724:LYS:HD3	1:C:760:ARG:NH1	2.19	0.57
2:F:46:LYS:HG3	2:F:113:VAL:HG21	1.86	0.57
1:B:777:ASP:OD1	1:B:819:ARG:NH1	2.28	0.57
1:B:889:LEU:HD22	1:B:933:PHE:HD2	1.69	0.57
1:A:920:TYR:CE2	1:A:944:VAL:HA	2.40	0.57
1:D:731:GLU:O	1:D:735:LYS:NZ	2.38	0.57
1:A:19:PHE:HA	1:A:22:LEU:HG	1.86	0.57
1:B:810:HIS:C	1:B:810:HIS:HD1	2.08	0.57
2:E:88:HIS:HB3	2:E:91:THR:O	2.05	0.57
2:F:14:LEU:HD11	2:F:23:PHE:HD2	1.69	0.57
1:A:802:ARG:NH1	1:A:870:ARG:HE	2.03	0.57
1:B:959:LEU:HD12	1:B:984:LEU:HD11	1.86	0.57
1:D:874:ILE:HD12	1:D:874:ILE:O	2.04	0.57
1:A:741:LEU:HA	1:A:754:ARG:HD3	1.87	0.56
1:A:759:GLU:O	1:A:762:THR:OG1	2.18	0.56
1:B:94:VAL:HG23	1:B:95:LYS:HG2	1.87	0.56
2:E:44:PHE:HD2	2:E:64:ILE:HD11	1.70	0.56
1:D:867:ASN:OD1	1:D:870:ARG:NH2	2.38	0.56
1:A:793:GLU:OE2	1:A:801:SER:OG	2.22	0.56
2:E:46:LYS:HG3	2:E:113:VAL:HG21	1.86	0.56
1:C:508:THR:HG23	1:C:511:PHE:H	1.71	0.56
2:F:99:VAL:HG13	2:F:112:ILE:HG13	1.88	0.56
1:A:222:ASP:O	1:A:226:ASN:ND2	2.35	0.56
1:C:56:TYR:CZ	1:C:135:ASP:HB3	2.41	0.56
1:C:514:ARG:HA	1:C:517:ARG:HH12	1.70	0.56
1:D:319:LEU:HD11	1:D:333:VAL:HG21	1.88	0.56
1:D:845:LEU:O	1:D:850:LYS:NZ	2.34	0.56
1:B:319:LEU:HD11	1:B:333:VAL:HG21	1.88	0.56
1:C:297:GLN:HE22	1:D:521:ASN:HD21	1.54	0.56
1:C:739:ALA:HA	1:C:743:TYR:HD2	1.71	0.56
1:B:30:ILE:HG23	1:B:293:LEU:HD23	1.89	0.55
1:D:839:PHE:CE2	1:D:857:LYS:HD3	2.41	0.55
2:F:54:ASN:HB3	2:F:58:ASP:HB2	1.88	0.55
1:A:202:ASN:OD1	1:B:202:ASN:ND2	2.39	0.55
1:C:914:SER:HB3	1:C:939:GLN:HG2	1.87	0.55



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:103:SER:HA	2:E:111:PRO:HG2	1.88	0.55
1:C:296:SER:HB3	1:C:301:PHE:HZ	1.71	0.55
2:F:99:VAL:O	2:F:103:SER:OG	2.19	0.55
1:C:101:ASP:OD1	1:C:180:GLY:N	2.39	0.55
1:D:291:ASP:O	1:D:295:GLU:HG2	2.06	0.55
1:D:359:ARG:NH1	1:D:362:GLU:OE1	2.39	0.55
2:F:94:ASP:OD1	2:F:96:THR:OG1	2.20	0.55
1:B:544:PHE:HD2	1:B:550:PHE:HB2	1.72	0.55
1:D:767:LEU:HB2	1:D:811:PHE:CG	2.42	0.55
1:A:364:LYS:O	1:A:370:ARG:NH2	2.30	0.55
1:D:581:ASP:OD1	1:D:622:LYS:NZ	2.28	0.55
1:C:324:TYR:OH	1:C:590:ASP:OD1	2.20	0.55
1:C:930:MET:HA	1:C:933:PHE:HD2	1.72	0.55
1:A:149:PHE:HB3	1:A:167:LEU:HB2	1.88	0.54
1:A:608:PHE:O	1:A:612:ILE:HG12	2.07	0.54
1:B:155:GLU:OE2	1:B:197:TYR:HA	2.07	0.54
1:A:801:SER:HA	1:A:804:TYR:CD1	2.42	0.54
1:B:724:LYS:HE3	2:E:124:PRO:HA	1.89	0.54
1:D:449:GLU:CD	1:D:449:GLU:H	2.08	0.54
1:D:966:LEU:HD12	2:F:59:PHE:HB2	1.89	0.54
1:A:80:SER:HB3	1:A:83:GLU:HG2	1.89	0.54
1:A:755:TYR:HB2	1:A:804:TYR:CZ	2.43	0.54
1:B:675:LYS:O	1:B:675:LYS:HD3	2.07	0.54
1:C:661:ILE:HD11	1:C:717:LYS:HG2	1.88	0.54
1:C:801:SER:HA	1:C:804:TYR:CD1	2.42	0.54
1:D:967:LEU:HD22	1:D:1005:ILE:HD13	1.88	0.54
1:B:913:MET:HA	1:B:916:PHE:CD2	2.43	0.54
1:B:776:ASP:OD1	1:B:819:ARG:NH1	2.41	0.54
1:A:866:MET:HG2	1:A:919:TRP:HH2	1.73	0.54
1:B:147:LYS:HD3	1:B:149:PHE:HE1	1.73	0.54
1:C:296:SER:HB3	1:C:301:PHE:CZ	2.43	0.54
1:C:884:LEU:HA	1:C:887:GLU:HG2	1.90	0.54
2:F:27:VAL:HG12	2:F:88:HIS:HA	1.89	0.54
1:C:454:LEU:O	1:C:458:ILE:HG13	2.07	0.54
1:B:755:TYR:HB2	1:B:804:TYR:CZ	2.43	0.54
1:C:142:CYS:HG	1:C:149:PHE:HD2	1.56	0.54
1:A:852:HIS:O	1:A:855:SER:OG	2.21	0.54
2:E:52:ARG:NH2	2:E:58:ASP:OD2	2.41	0.54
1:D:319:LEU:HD13	1:D:325:ILE:HG12	1.88	0.54
1:D:364:LYS:NZ	1:D:394:ILE:O	2.38	0.54
1:A:480:ARG:NH2	1:A:546:SER:O	2.41	0.53



	to do pago	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:394:ILE:HD12	1:D:395:CYS:N	2.23	0.53	
1:A:433:GLU:N	1:A:433:GLU:OE1	2.39	0.53	
1:A:664:ILE:O	1:A:668:GLU:HG3	2.08	0.53	
1:B:611:TYR:O	1:B:615:SER:OG	2.25	0.53	
1:B:954:PHE:CE1	1:B:983:VAL:HG11	2.43	0.53	
1:C:804:TYR:O	1:C:808:ILE:HG13	2.09	0.53	
1:C:863:ASN:O	1:C:867:ASN:ND2	2.41	0.53	
1:D:661:ILE:HA	1:D:664:ILE:HD12	1.91	0.53	
1:A:692:ALA:O	1:A:696:THR:HG23	2.08	0.53	
1:C:646:PHE:HB2	1:C:677:ARG:HG2	1.90	0.53	
1:C:655:ILE:HA	1:C:659:PHE:CD1	2.43	0.53	
1:A:818:LYS:HE2	1:A:819:ARG:HH22	1.74	0.53	
1:B:364:LYS:NZ	1:B:394:ILE:O	2.40	0.53	
2:E:99:VAL:O	2:E:103:SER:OG	2.24	0.53	
1:C:364:LYS:NZ	1:C:394:ILE:O	2.37	0.53	
1:D:669:ARG:HD2	2:F:121:TRP:HE3	1.74	0.53	
1:A:147:LYS:NZ	1:A:165:ARG:HE	2.06	0.53	
1:A:561:LEU:HD12	1:A:584:VAL:HG23	1.90	0.53	
1:B:966:LEU:HD12	2:E:59:PHE:HB2	1.91	0.53	
1:C:320:PHE:HE1	1:C:387:PHE:HB2	1.74	0.53	
1:A:728:LEU:O	1:A:765:ASN:ND2	2.42	0.53	
1:B:916:PHE:HD1	1:B:919:TRP:HZ3	1.56	0.53	
1:C:839:PHE:HE1	1:C:873:LEU:HD22	1.74	0.53	
1:A:419:ASP:O	1:A:423:LYS:HG2	2.09	0.52	
1:A:696:THR:HG22	1:A:743:TYR:HD2	1.73	0.52	
2:E:43:TYR:CE1	2:E:67:PHE:HB2	2.44	0.52	
1:C:589:TYR:OH	1:C:651:ASP:OD1	2.27	0.52	
1:C:751:ILE:O	1:C:804:TYR:OH	2.24	0.52	
1:B:967:LEU:HB3	1:B:1005:ILE:HD11	1.91	0.52	
1:B:13:GLU:O	1:B:17:GLU:HG3	2.10	0.52	
1:B:772:ILE:HG12	1:B:808:ILE:HG23	1.92	0.52	
2:E:51:TYR:CD2	2:E:123:HIS:HD2	2.27	0.52	
1:C:534:GLU:HG2	1:C:535:PHE:N	2.24	0.52	
1:B:839:PHE:CE2	1:B:857:LYS:HG3	2.45	0.52	
2:E:20:ILE:O	2:E:20:ILE:HD12	2.09	0.52	
1:D:835:ILE:HG22	1:D:857:LYS:HE3	1.91	0.52	
1:B:767:LEU:HG	1:B:772:ILE:HG13	1.91	0.52	
1:C:772:ILE:HD12	1:C:775:ILE:HD12	1.92	0.52	
1:D:250:PRO:HA	1:D:285:ARG:NH1	2.25	0.52	
1:D:912:TYR:HB3	1:D:916:PHE:CE1	2.41	0.52	
1:A:959:LEU:HD13	1:A:984:LEU:HD13	1.92	0.51	



	to us page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:57:PRO:HA	1:C:61:ARG:NH1	2.24	0.51
1:C:256:GLU:N	1:C:256:GLU:OE1	2.39	0.51
1:C:557:LYS:O	1:C:561:LEU:HD12	2.10	0.51
1:A:737:VAL:HG13	1:A:741:LEU:HD23	1.92	0.51
1:B:54:SER:O	1:B:54:SER:OG	2.28	0.51
1:B:863:ASN:HD21	2:E:77:ASN:HA	1.76	0.51
1:A:728:LEU:N	1:A:765:ASN:HD21	2.06	0.51
1:B:832:GLN:O	1:B:835:ILE:HG13	2.10	0.51
1:D:163:SER:OG	1:D:164:SER:N	2.44	0.51
1:D:960:LYS:HE2	1:D:996:TYR:CE1	2.46	0.51
1:C:89:GLN:NE2	1:C:93:ASN:OD1	2.43	0.51
1:D:695:ILE:HG12	1:D:744:PHE:CE1	2.45	0.51
1:D:755:TYR:CE1	1:D:759:GLU:HB2	2.45	0.51
1:A:738:LYS:HD2	1:A:742:PHE:HD2	1.75	0.51
1:D:544:PHE:HD2	1:D:550:PHE:HB2	1.75	0.51
1:C:376:LYS:O	1:C:380:ARG:HG3	2.11	0.51
1:C:447:ARG:HB3	1:C:450:GLU:HG3	1.93	0.51
1:C:751:ILE:HD12	1:C:752:GLY:N	2.26	0.51
1:C:913:MET:SD	1:C:913:MET:N	2.81	0.51
1:C:310:ASP:OD2	1:C:377:GLN:NE2	2.43	0.51
1:C:755:TYR:HD2	1:C:799:LEU:HD13	1.76	0.51
1:B:17:GLU:O	1:B:21:MET:HG2	2.11	0.51
1:B:56:TYR:CZ	1:B:135:ASP:HB3	2.46	0.51
1:B:561:LEU:HD11	1:B:584:VAL:HG11	1.92	0.51
1:D:29:CYS:O	1:D:33:ILE:HD12	2.11	0.51
1:A:976:MET:O	1:A:980:VAL:HG22	2.11	0.51
1:B:10:ARG:H	1:B:10:ARG:HE	1.59	0.51
1:B:83:GLU:HB3	1:B:87:ILE:HD12	1.92	0.51
1:B:284:GLU:H	1:B:284:GLU:CD	2.15	0.51
1:B:674:ASP:OD1	1:B:674:ASP:N	2.38	0.51
1:B:978:HIS:HA	1:B:981:ILE:HG22	1.93	0.51
1:D:602:SER:HA	1:D:605:PHE:HD2	1.75	0.51
1:A:447:ARG:HB3	1:A:450:GLU:HG3	1.91	0.50
1:A:460:LEU:HD21	1:B:144:LYS:HE2	1.93	0.50
1:A:946:PRO:HB2	1:A:975:HIS:HB3	1.93	0.50
1:C:802:ARG:HB3	1:C:840:LYS:HB3	1.94	0.50
1:D:828:THR:O	1:D:835:ILE:HD11	2.10	0.50
1:A:681:GLN:HG2	1:A:726:VAL:HG13	1.93	0.50
1:B:186:LYS:NZ	1:B:189:ASP:OD1	2.44	0.50
1:B:419:ASP:O	1:B:423:LYS:HG2	2.12	0.50
1:C:841:LEU:HB3	$1:\overline{C:844:LEU:HD12}$	1.92	0.50



	to us page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:685:GLU:O	1:D:689:VAL:HG13	2.12	0.50
2:F:44:PHE:HB3	2:F:64:ILE:HD11	1.91	0.50
1:A:741:LEU:HD21	1:A:758:LEU:HD13	1.93	0.50
1:C:31:LYS:O	1:C:35:GLU:HG3	2.12	0.50
1:C:473:LEU:HD22	1:C:600:LEU:HD21	1.94	0.50
1:D:885:ILE:HG23	1:D:916:PHE:CD2	2.46	0.50
1:A:967:LEU:HA	1:A:970:ILE:HG22	1.93	0.50
1:B:373:LEU:HD23	1:B:377:GLN:HB3	1.94	0.50
1:B:997:LEU:O	1:B:1001:MET:HB2	2.11	0.50
1:A:547:ASP:OD1	1:A:547:ASP:N	2.42	0.50
1:A:775:ILE:HB	1:A:808:ILE:HD11	1.93	0.50
1:B:349:HIS:CE1	1:B:350:LYS:HG3	2.46	0.50
2:E:123:HIS:ND1	2:E:124:PRO:HD2	2.26	0.50
2:E:123:HIS:CD2	2:E:125:GLN:HB2	2.47	0.50
1:D:473:LEU:HD22	1:D:600:LEU:HD21	1.93	0.50
1:B:671:CYS:SG	1:B:672:SER:N	2.85	0.50
1:C:589:TYR:HE1	1:C:654:ASN:HD21	1.59	0.50
1:C:647:MET:O	1:C:679:GLY:N	2.36	0.50
1:D:817:SER:O	1:D:821:SER:OG	2.27	0.50
1:A:985:LYS:HA	1:B:1001:MET:HE3	1.94	0.50
1:B:724:LYS:HB2	1:B:760:ARG:HB3	1.94	0.50
1:B:942:PHE:HE1	1:B:976:MET:HB2	1.77	0.50
2:E:52:ARG:HH21	2:E:54:ASN:CA	2.16	0.50
1:D:22:LEU:HD21	1:D:292:LEU:HD21	1.94	0.50
1:D:47:GLY:O	1:D:133:ASN:ND2	2.35	0.50
1:D:631:ILE:HD12	1:D:636:PHE:H	1.77	0.50
2:F:106:ILE:HD11	2:F:111:PRO:HG3	1.94	0.50
1:C:987:ARG:HE	1:C:987:ARG:HA	1.77	0.49
1:D:270:ASP:HB3	1:D:273:SER:HB3	1.93	0.49
1:D:588:LEU:HD12	1:D:615:SER:OG	2.12	0.49
1:D:691:ILE:O	1:D:695:ILE:HD12	2.12	0.49
1:A:791:TYR:O	1:A:833:LYS:NZ	2.44	0.49
1:A:620:ILE:HD11	1:A:655:ILE:HD11	1.94	0.49
2:E:99:VAL:HG22	2:E:112:ILE:HD12	1.93	0.49
2:E:14:LEU:HD11	2:E:23:PHE:HB3	1.93	0.49
1:B:863:ASN:ND2	2:E:77:ASN:HA	2.28	0.49
1:D:671:CYS:SG	1:D:672:SER:N	2.85	0.49
1:D:739:ALA:HA	1:D:743:TYR:HD2	1.77	0.49
1:D:787:ILE:N	1:D:834:GLN:HE21	2.11	0.49
1:D:812:GLU:HG2	1:D:815:PHE:HB2	1.94	0.49
1:B:720:LEU:HB3	1:B:757:TRP:HD1	1.77	0.49



	A A A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (\AA)
1:A:772:ILE:HG23	1:A:808:ILE:HD12	1.94	0.49
1:B:308:VAL:HG13	1:B:356:TYR:HB2	1.94	0.49
1:C:489:VAL:HG21	1:C:512:LEU:HD21	1.94	0.49
1:C:136:ASN:O	1:C:140:THR:HG23	2.12	0.49
1:D:136:ASN:O	1:D:140:THR:HG23	2.13	0.49
1:D:432:ILE:HG12	1:D:458:ILE:HG23	1.95	0.49
1:D:661:ILE:HG22	1:D:665:LYS:HE2	1.94	0.49
1:A:878:THR:H	1:A:881:HIS:CD2	2.31	0.49
1:C:305:ASP:OD2	1:C:359:ARG:NH2	2.44	0.49
1:D:14:LYS:HA	1:D:17:GLU:HG3	1.95	0.49
1:A:818:LYS:HB2	1:A:819:ARG:HH22	1.78	0.48
1:B:368:ASP:OD1	1:B:368:ASP:N	2.46	0.48
2:E:121:TRP:HA	2:E:126:PHE:CD2	2.48	0.48
1:D:537:LYS:HE2	1:D:537:LYS:HB3	1.61	0.48
1:D:888:TYR:O	1:D:891:THR:OG1	2.29	0.48
1:D:955:ILE:HD12	1:D:958:TRP:HE1	1.78	0.48
1:B:122:LEU:HD11	1:B:142:CYS:SG	2.53	0.48
1:B:589:TYR:OH	1:B:651:ASP:OD2	2.30	0.48
1:D:56:TYR:CZ	1:D:135:ASP:HB3	2.49	0.48
1:D:777:ASP:O	1:D:781:LEU:HD23	2.13	0.48
2:F:106:ILE:HD12	2:F:107:SER:N	2.28	0.48
1:A:184:VAL:HG13	1:A:189:ASP:HB3	1.95	0.48
1:B:553:ASP:O	1:B:557:LYS:HG3	2.13	0.48
1:B:867:ASN:OD1	1:B:870:ARG:NH2	2.46	0.48
1:C:424:PHE:O	1:C:438:LYS:NZ	2.42	0.48
1:C:836:ASP:HA	1:C:857:LYS:HZ3	1.78	0.48
1:C:842:LEU:HB3	1:C:843:PRO:HD2	1.96	0.48
1:D:755:TYR:CD2	1:D:799:LEU:HD21	2.47	0.48
1:C:613:ARG:HA	1:C:659:PHE:CE1	2.48	0.48
1:D:781:LEU:O	1:D:785:LYS:HG2	2.14	0.48
1:A:938:ASP:HB2	1:A:958:TRP:HH2	1.78	0.48
1:B:462:SER:HB3	1:B:471:TYR:HB2	1.96	0.48
1:B:973:ASN:C	1:B:975:HIS:H	2.16	0.48
1:C:31:LYS:HG3	1:C:301:PHE:CD2	2.49	0.48
1:D:414:TYR:O	1:D:657:ARG:NH2	2.40	0.48
1:D:804:TYR:O	1:D:808:ILE:HG13	2.13	0.48
1:C:230:ASN:O	1:C:233:ARG:HG2	2.13	0.48
1:C:688:LEU:O	1:C:691:ILE:HG22	2.13	0.48
1:A:37:SER:OG	1:A:124:MET:O	2.28	0.48
1:A:92:TYR:CG	1:A:186:LYS:HE2	2.48	0.48
1:A:142:CYS:HG	1:A:149:PHE:HD2	1.59	0.48



	A h o	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:684:ILE:HG21	1:A:726:VAL:HG21	1.94	0.48	
1:A:954:PHE:HE2	1:A:980:VAL:HG12	1.79	0.48	
1:B:730:GLU:HA	1:B:730:GLU:OE1	2.13	0.48	
1:B:950:ASP:HB3	1:B:953:LYS:HZ1	1.78	0.48	
1:C:733:LEU:HD12	1:C:765:ASN:HD22	1.78	0.48	
1:A:713:ILE:HG12	1:A:748:ASP:OD2	2.14	0.48	
1:B:9:LYS:O	1:B:13:GLU:HG3	2.13	0.48	
1:B:9:LYS:NZ	1:B:9:LYS:HB3	2.28	0.48	
1:B:916:PHE:HA	1:B:919:TRP:CE3	2.48	0.48	
1:D:120:LYS:HB3	1:D:290:MET:HE2	1.95	0.48	
1:D:548:ASN:OD1	1:D:548:ASN:N	2.44	0.48	
1:D:831:LYS:O	1:D:835:ILE:HD12	2.14	0.48	
1:D:960:LYS:NZ	2:F:21:ASN:HB3	2.29	0.48	
1:B:338:TYR:CZ	1:B:357:MET:HB2	2.49	0.47	
1:C:492:PHE:HA	1:C:496:GLY:HA3	1.96	0.47	
1:C:685:GLU:O	1:C:689:VAL:HG13	2.14	0.47	
1:D:368:ASP:N	1:D:368:ASP:OD1	2.46	0.47	
1:D:705:ASN:O	1:D:709:TYR:N	2.42	0.47	
1:B:779:LEU:HD21	1:B:804:TYR:HB2	1.96	0.47	
1:C:666:ASN:OD1	1:C:669:ARG:NH2	2.47	0.47	
1:C:835:ILE:HG22	1:C:857:LYS:HD3	1.96	0.47	
1:A:300:LYS:HB2	1:A:302:ILE:HG13	1.96	0.47	
1:C:51:SER:OG	1:C:135:ASP:OD2	2.23	0.47	
1:D:38:ARG:HH21	1:D:297:GLN:HA	1.79	0.47	
1:D:669:ARG:HH11	2:F:121:TRP:HE3	1.61	0.47	
1:D:975:HIS:O	1:D:976:MET:HB3	2.14	0.47	
1:B:912:TYR:HA	1:B:915:THR:HG23	1.96	0.47	
1:D:669:ARG:HD2	2:F:121:TRP:CE3	2.50	0.47	
1:D:962:TYR:CD2	1:D:966:LEU:HD22	2.49	0.47	
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.80	0.47	
1:C:298:GLU:H	1:C:298:GLU:CD	2.16	0.47	
1:D:620:ILE:HD13	1:D:667:LEU:HD21	1.96	0.47	
1:A:92:TYR:HE1	1:A:97:GLU:HG3	1.80	0.47	
1:A:809:LYS:HD3	1:A:844:LEU:HD23	1.96	0.47	
1:A:836:ASP:HB3	1:A:857:LYS:NZ	2.29	0.47	
1:B:90:ILE:HD13	1:C:260:TYR:CG	2.49	0.47	
1:B:432:ILE:HG13	1:B:458:ILE:HG23	1.97	0.47	
1:B:700:SER:HB2	1:B:743:TYR:CE2	2.49	0.47	
1:C:477:ASN:HD21	1:C:600:LEU:HA	1.80	0.47	
1:C:708:PHE:CE1	1:C:712:PHE:HB2	2.50	0.47	
1:D:30:ILE:HG12	1:D:293:LEU:HD12	1.96	0.47	



	bous page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:291:ASP:HA	1:D:294:ILE:HB	1.96	0.47	
1:D:359:ARG:HD2	1:D:359:ARG:HA	1.80	0.47	
2:F:31:ILE:HG22	2:F:83:ILE:HA	1.96	0.47	
1:A:827:LEU:HD13	1:A:835:ILE:HG23	1.97	0.47	
1:B:705:ASN:O	1:B:709:TYR:N	2.40	0.47	
2:E:105:ARG:HG2	2:E:105:ARG:HH11	1.79	0.47	
2:F:29:PHE:N	2:F:42:CYS:O	2.46	0.47	
1:B:115:ASN:ND2	1:B:117:ILE:HB	2.30	0.47	
1:B:347:VAL:HG22	1:B:397:ALA:HB2	1.96	0.47	
1:B:994:LYS:HA	1:B:994:LYS:HD3	1.62	0.47	
1:D:23:ASP:OD1	1:D:24:ASN:N	2.48	0.47	
1:D:116:PRO:HB2	1:D:120:LYS:NZ	2.29	0.47	
1:A:970:ILE:HD11	1:A:976:MET:HE2	1.96	0.47	
1:C:313:TYR:HA	1:C:384:LEU:HD21	1.97	0.47	
1:A:446:GLY:HA3	1:A:708:PHE:HB2	1.97	0.46	
1:D:43:VAL:HB	1:D:213:ILE:HD13	1.96	0.46	
1:D:446:GLY:HA3	1:D:708:PHE:HB2	1.96	0.46	
1:A:668:GLU:O	1:A:994:LYS:NZ	2.46	0.46	
2:E:11:THR:O	2:E:11:THR:OG1	2.30	0.46	
1:C:514:ARG:HA	1:C:517:ARG:NH1	2.31	0.46	
1:C:772:ILE:CD1	1:C:808:ILE:HG23	2.41	0.46	
1:A:65:LYS:NZ	1:A:69:GLU:OE2	2.47	0.46	
1:A:758:LEU:HD21	1:A:775:ILE:HD13	1.98	0.46	
1:B:155:GLU:OE1	1:B:199:LEU:HB2	2.15	0.46	
1:B:617:SER:HA	1:B:667:LEU:HD21	1.97	0.46	
1:C:169:LYS:HD2	1:C:173:ASP:HB3	1.96	0.46	
1:D:407:ILE:HD11	1:D:593:ARG:HG3	1.98	0.46	
1:D:930:MET:HG3	1:D:940:TYR:OH	2.14	0.46	
1:A:25:ASN:OD1	1:A:26:VAL:N	2.49	0.46	
1:B:517:ARG:O	1:B:520:THR:HG22	2.16	0.46	
1:B:622:LYS:O	1:B:626:GLU:HG2	2.15	0.46	
1:C:146:GLY:O	1:D:475:GLN:NE2	2.48	0.46	
1:B:691:ILE:O	1:B:695:ILE:HG22	2.16	0.46	
1:B:787:ILE:HG13 1:B:788:ASP:I		2.31	0.46	
1:B:956:PRO:HG2 1:B:987:ARG:HD3		1.98	0.46	
1:C:698:GLN:HE22	1:C:705:ASN:H	1.64	0.46	
1:A:581:ASP:HB2	1:A:619:LEU:HD23	1.98	0.46	
1:C:368:ASP:OD1	1:C:369:GLU:N	2.49	0.46	
2:F:21:ASN:HD21	2:F:108:SER:HB3	1.81	0.46	
1:A:363:LEU:HD23	1:A:373:LEU:HD11	1.98	0.46	
1:B:827:LEU:HD21	1:B:834:GLN:HB3	1.97	0.46	



	ious page	Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:D:678:PHE:HZ	1:D:722:PHE:HE2	1.64	0.46	
1:C:930:MET:HB2	1:C:940:TYR:OH	2.16	0.46	
1:D:749:LEU:HD22	1:D:754:ARG:HA	1.97	0.46	
1:D:882:GLU:HG2	1:D:927:ASN:HB2	1.98	0.46	
1:D:885:ILE:HG23	1:D:916:PHE:HD2	1.80	0.46	
1:D:962:TYR:HD2	1:D:966:LEU:HD22	1.80	0.46	
1:A:581:ASP:OD2	1:A:622:LYS:HG2	2.16	0.46	
1:B:537:LYS:HB3	1:B:537:LYS:HE2	1.62	0.46	
1:B:812:GLU:HG2	1:B:815:PHE:HB2	1.97	0.46	
1:C:984:LEU:O	1:C:988:VAL:HG22	2.16	0.46	
1:C:938:ASP:HB2	1:C:958:TRP:HH2	1.80	0.46	
1:D:139:ASP:OD2	1:D:169:LYS:NZ	2.49	0.46	
1:D:338:TYR:CZ	1:D:357:MET:HB2	2.51	0.46	
1:D:969:LYS:HE2	1:D:969:LYS:HB2	1.67	0.46	
1:A:529:ASN:O	1:A:536:GLN:NE2	2.49	0.45	
1:A:747:ARG:HG2	1:A:748:ASP:OD1	2.16	0.45	
1:B:449:GLU:OE2	1:B:449:GLU:N	2.30	0.45	
1:C:511:PHE:HD1	1:C:514:ARG:HH22	1.64	0.45	
1:D:912:TYR:O	1:D:916:PHE:HD1	1.98	0.45	
1:B:655:ILE:O	1:B:659:PHE:HB2	2.17	0.45	
1:B:771:ILE:O	1:B:775:ILE:HG13	2.15	0.45	
1:B:877:PHE:HB3	1:B:882:GLU:OE1	2.16	0.45	
1:C:750:ASP:OD1	1:C:752:GLY:N	2.47	0.45	
1:D:150:SER:OG	1:D:165:ARG:O 2.3		0.45	
1:B:90:ILE:O	1:B:94:VAL:HG22	2.16	0.45	
1:B:663:ASP:OD1	1:B:663:ASP:N	2.49	0.45	
1:B:810:HIS:C	1:B:810:HIS:ND1	2.69	0.45	
1:C:313:TYR:O	1:C:317:SER:OG	2.25	0.45	
1:D:959:LEU:H	1:D:959:LEU:HD22	1.80	0.45	
1:A:717:LYS:HE3	1:A:717:LYS:HB3	1.69	0.45	
1:A:955:ILE:HB	1:A:958:TRP:CE2	2.51	0.45	
1:B:945:ASP:N	1:B:945:ASP:OD1	2.50	0.45	
1:C:152:ILE:HG23	1:C:157:ASP:HB2	1.98	0.45	
1:C:787:ILE:HA	1:C:834:GLN:CD	2.36	0.45	
1:A:705:ASN:HB3	1:A:708:PHE:HB3	1.99	0.45	
1:C:375:LYS:HG3	1:C:376:LYS:N	2.32	0.45	
1:D:809:LYS:HD2	1:D:809:LYS:HA	1.77	0.45	
1:A:432:ILE:HG13	1:A:458:ILE:HG23	1.98	0.45	
1:A:797:ASN:ND2	1:A:799:LEU:HD12	2.32	0.45	
1:B:697:LYS:HE3	1:B:697:LYS:HB2	1.74	0.45	
1:B:809:LYS:HG3	1:B:843:PRO:HB2	1.98	0.45	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:0:578:MET:HEI	1:U:580:SER:HA	1.98	0.45
1:D:123:ALA:HA	1:D:145:ARG:HH21	1.81	0.45
1:D:617:SER:O	1:D:621:GLU:HG2	2.17	0.45
1:D:976:MET:O	1:D:980:VAL:HG22	2.17	0.45
1:D:772:ILE:HG12	1:D:808:ILE:HG23	1.99	0.45
1:D:839:PHE:CE2	1:D:853:LEU:HG	2.52	0.45
2:F:95:VAL:O	2:F:99:VAL:HG23	2.17	0.45
2:E:105:ARG:HG2	2:E:105:ARG:NH1	2.31	0.45
1:C:974:LYS:HD2	1:C:974:LYS:O	2.17	0.45
1:D:956:PRO:HG3	1:D:983:VAL:HG22	1.99	0.45
2:F:48:PHE:HD1	2:F:50:PRO:HD3	1.81	0.45
1:C:673:ILE:H	1:C:673:ILE:HD12	1.82	0.45
1:D:339:HIS:CE1	1:D:349:HIS:HB2	2.52	0.45
1:B:174:PHE:CD1	1:B:178:PHE:HA	2.51	0.44
1:B:805:GLY:HA2	1:B:808:ILE:HD12	2.00	0.44
1:C:561:LEU:HD13	1:C:584:VAL:HG23	1.99	0.44
1:D:94:VAL:HG23	1:D:95:LYS:HG2	1.99	0.44
1:D:751:ILE:O	1:D:804:TYR:OH	2.31	0.44
1:B:682:GLU:H	1:B:682:GLU:CD	2.20	0.44
1:C:523:ASN:HB3	1:C:526:ASP:OD1	2.18	0.44
1:D:919:TRP:N	1:D:919:TRP:CD1	2.83	0.44
1:A:313:TYR:HA	1:A:384:LEU:HD21	1.98	0.44
1:A:1004:PHE:CZ	1:B:985:LYS:HD3	2.52	0.44
1:C:887:GLU:HG3	1:C:888:TYR:N	2.32	0.44
1:D:594:PHE:O	1:D:598:ASN:HB2	2.17	0.44
1:A:818:LYS:HB2	1:A:819:ARG:CZ	2.47	0.44
1:B:467:ASN:N	1:B:467:ASN:ND2	2.62	0.44
1:B:594:PHE:O	1:B:598:ASN:HB2	2.17	0.44
1:B:630:ASP:O	1:B:634:LEU:N	2.34	0.44
1:B:824:THR:O	1:B:827:LEU:HB2	2.18	0.44
1:C:145:ARG:HG2	1:C:147:LYS:HG2	1.99	0.44
1:D:880:GLU:OE2	1:D:881:HIS:ND1	2.51	0.44
2:E:32:VAL:HG12	2:E:38:GLU:HG2	2.00	0.44
1:C:1004:PHE:CE2	1:D:985:LYS:HD3	2.53	0.44
2:F:20:ILE:HG23	2:F:48:PHE:CD2	2.53	0.44
1:B:886:ILE:O	1:B:890:GLU:HG2	2.18	0.44
1:C:672:SER:O	1:C:672:SER:OG	2.30	0.44
1:C:772:ILE:HD12	1:C:772:ILE:HA	1.76	0.44
1:C:793:GLU:OE2	1:C:801:SEB:OG	2.35	0.44
1.C.886.ILE.O	1.C.890.GLU.HG3	2.18	0.44
1.D.835.ILE.CG2	1.D.857.LYS.HE3	2.48	0.44



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:B:981:ILE:HGI3	1:B:1000:LEU:HD21	2.00	0.44
1:0:370:LYS:0	1:C:379:GLU:HG2	2.17	0.44
1:C:877:PHE:HB3	1:C:882:GLU:OE1	2.17	0.44
1:D:386:ASN:HA	1:D:389:GLU:OE1	2.18	0.44
1:A:432:ILE:HD12	1:A:432:ILE:HA	1.87	0.44
1:A:531:MET:SD	1:A:532:PRO:HD2	2.58	0.44
1:A:980:VAL:CG2	1:A:1005:ILE:HG22	2.47	0.44
1:B:936:MET:SD	1:B:936:MET:N	2.91	0.44
1:C:617:SER:O	1:C:621:GLU:HG3	2.17	0.44
1:D:22:LEU:HD12	1:D:22:LEU:HA	1.87	0.44
1:D:324:TYR:OH	1:D:590:ASP:OD1	2.17	0.44
1:D:747:ARG:H	1:D:747:ARG:HG2	1.56	0.44
1:A:470:VAL:O	1:A:474:SER:OG	2.30	0.44
1:B:665:LYS:HD3	2:E:121:TRP:CD2	2.53	0.44
1:B:809:LYS:HD2	1:B:809:LYS:HA	1.68	0.44
1:D:79:TYR:HB3	1:D:84:TYR:CE1	2.50	0.44
1:D:655:ILE:O	1:D:659:PHE:HB2	2.18	0.44
1:D:885:ILE:HG12	1:D:916:PHE:CE2	2.52	0.44
1:D:964:ASP:OD1	1:D:965:LYS:N	2.51	0.44
1:D:687:TYR:OH	1:D:715:GLU:OE2	2.32	0.43
1:A:685:GLU:OE1	1:A:728:LEU:HA	2.19	0.43
1:B:270:ASP:O	1:B:274:LEU:HG	2.18	0.43
1:C:861:ASN:OD1	1:C:863:ASN:N	2.42	0.43
1:D:417:LYS:HD3	1:D:417:LYS:HA	1.63	0.43
1:D:675:LYS:HA	1:D:675:LYS:HD2	1.75	0.43
1:D:696:THR:O	1:D:700:SER:HB3	2.18	0.43
1:A:174:PHE:CD1	1:A:178:PHE:HA	2.53	0.43
1:C:374:SER:OG	1:C:375:LYS:N	2.51	0.43
1:A:565:VAL:O	1:A:569:MET:HG3	2.19	0.43
1:A:797:ASN:HD22	1:A:799:LEU:HD12	1.84	0.43
1:A:834:GLN:O	1:A:838:LEU:HD12	2.18	0.43
2:E:20:ILE:HD13	2:E:22:THR:HG23	1.99	0.43
1:C:803:ASP:HA	1:C:870:ARG:HH22	1.82	0.43
1:C:879:PRO:HA	1:C:882:GLU:OE2	2.18	0.43
1:A:514:ARG:O	1:A:518:GLU:HG3	2.19	0.43
1:A:779:LEU:HD13	1:A:779:LEU:HA	1.90	0.43
1:C:293:LEU:HD23	1:C:293:LEU:HA	1.91	0.43
1:C:832:GLN:HA	1:C:835:ILE:HD12	1.99	0.43
1:A:43:VAL·HB	1:A:213:ILE·HD13	2.01	0.43
1:A:820:LEU:O	1:A:823:ILE:HG12	2.18	0.43
1:B:168:LEU:HD11	1:B:200:ILE:HG23	2.01	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:763:LYS:HB2	2:E:124:PRO:HB2	2.00	0.43	
1:C:418:TYR:CD2	1:C:694:GLU:HG3	2.53	0.43	
1:C:581:ASP:OD1	1:C:581:ASP:N	2.52	0.43	
1:C:789:GLN:HA	1:C:833:LYS:HG3	2.00	0.43	
1:D:492:PHE:CE2	1:D:506:PRO:HG3	2.53	0.43	
1:A:54:SER:O	1:A:54:SER:OG	2.31	0.43	
1:A:802:ARG:HH22	1:A:870:ARG:NE	2.15	0.43	
2:E:31:ILE:HG21	2:E:81:PHE:HB2	2.01	0.43	
2:F:120:ASP:OD1	2:F:121:TRP:N	2.51	0.43	
1:A:834:GLN:OE1	1:A:838:LEU:HD11	2.18	0.43	
1:A:974:LYS:O	1:A:974:LYS:HG2	2.19	0.43	
1:A:1004:PHE:CE2	1:B:985:LYS:HD3	2.53	0.43	
1:B:117:ILE:HD13	1:B:120:LYS:HD2	2.01	0.43	
1:B:741:LEU:HA	1:B:754:ARG:HD3	2.01	0.43	
1:B:763:LYS:HB2	2:E:124:PRO:CB	2.49	0.43	
1:C:192:ASN:HB2	1:C:196:ASN:HD21	1.84	0.43	
1:C:343:ASN:ND2	1:C:345:THR:OG1	2.51	0.43	
1:C:422:LYS:O	1:C:426:GLU:HG2	2.19	0.43	
1:C:755:TYR:CD2	1:C:799:LEU:HD13	2.54	0.43	
1:D:551:LEU:HD11	1:D:608:PHE:HD1	1.83	0.43	
1:A:56:TYR:CZ	1:A:135:ASP:HB3	2.54	0.43	
1:A:374:SER:OG	1:A:375:LYS:N	2.51	0.43	
1:B:446:GLY:HA3	1:B:708:PHE:HB2	2.01	0.43	
1:B:942:PHE:HE2	1:B:954:PHE:CE2	2.37	0.43	
1:A:960:LYS:HG2	1:A:995:ARG:HG2	1.99	0.43	
1:B:942:PHE:CE1	1:B:976:MET:HE2	2.53	0.43	
1:B:962:TYR:CD2	1:B:966:LEU:HD22	2.54	0.43	
1:C:188:ASP:HA	1:C:191:LEU:HB2	2.01	0.43	
1:C:620:ILE:HD11	1:C:655:ILE:HD11	2.01	0.43	
1:C:628:THR:OG1	1:D:991:SER:O	2.35	0.43	
1:C:943:PHE:CE1	1:C:970:ILE:HD11	2.54	0.43	
1:D:831:LYS:H	1:D:831:LYS:HG2	1.59	0.43	
1:A:229:LEU:HD21	1:A:266:LEU:HG	2.00	0.42	
1:B:184:VAL:HG13	1:B:189:ASP:HB3	2.00	0.42	
1:B:551:LEU:HD11	1:B:608:PHE:HD1	1.84	0.42	
1:C:656:SER:O	1:C:715:GLU:HA	2.19	0.42	
1:C:976:MET:O	1:C:980:VAL:HG22	2.19	0.42	
1:A:53:LEU:C	1:A:115:ASN:HD21	2.23	0.42	
1:A:53:LEU:HD23	1:A:117:ILE:HD13	2.01	0.42	
1:A:570:SER:OG	1:B:669:ARG:HD3	2.18	0.42	
1:B:433:GLU:N	1:B:433:GLU:OE1	2.52	0.42	



	lous page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:E:97:GLU:OE1	2:E:97:GLU:N	2.44	0.42	
1:C:278:ASN:HB2	1:C:281:ASP:HB2	2.01	0.42	
1:C:416:GLY:HA2	1:C:418:TYR:CE1	2.54	0.42	
1:C:673:ILE:HD12	1:C:673:ILE:N	2.35	0.42	
1:C:816:ILE:O	1:C:818:LYS:NZ	2.39	0.42	
1:D:709:TYR:O	1:D:713:ILE:HG22	2.18	0.42	
1:A:260:TYR:CZ	1:A:264:LYS:HD2	2.55	0.42	
1:A:262:GLU:HA	1:A:266:LEU:O	2.19	0.42	
1:A:749:LEU:HD12	1:A:749:LEU:HA	1.91	0.42	
1:B:955:ILE:HB	1:B:958:TRP:NE1	2.33	0.42	
1:C:145:ARG:HE	1:C:147:LYS:HE2	1.83	0.42	
1:D:744:PHE:CE2	1:D:749:LEU:HD12	2.53	0.42	
1:D:980:VAL:O	1:D:983:VAL:HG12	2.18	0.42	
1:A:505:LYS:O	1:A:505:LYS:HD3	2.19	0.42	
1:A:737:VAL:HG11	1:A:771:ILE:HG23	2.00	0.42	
2:E:31:ILE:CG2	2:E:81:PHE:HB2	2.50	0.42	
1:C:833:LYS:HD2	1:C:833:LYS:HA	1.84	0.42	
1:D:220:LEU:HD23	1:D:220:LEU:HA	1.87	0.42	
1:B:152:ILE:HG23	1:B:157:ASP:HB2	2.02	0.42	
1:B:348:ARG:NH2	1:B:353:GLY:O	2.49	0.42	
1:B:456:SER:O	1:B:460:LEU:HD13	2.19	0.42	
1:C:504:TYR:CG	1:C:706:VAL:HG21	2.54	0.42	
1:D:313:TYR:HA	1:D:384:LEU:HD21	1.99	0.42	
1:D:945:ASP:OD1	1:D:945:ASP:N	2.53	0.42	
1:A:313:TYR:O	1:A:317:SER:OG	2.28	0.42	
1:A:861:ASN:OD1	1:A:863:ASN:N	2.43	0.42	
1:A:866:MET:O	1:A:869:ILE:HG22	2.19	0.42	
1:A:987:ARG:HA	1:A:987:ARG:NE	2.34	0.42	
1:B:974:LYS:O	1:B:974:LYS:HD3	2.20	0.42	
1:C:801:SER:HA	1:C:804:TYR:CE1	2.54	0.42	
1:D:954:PHE:CE1	1:D:983:VAL:HG11	2.54	0.42	
1:D:985:LYS:HB3	1:D:985:LYS:HE3	1.81	0.42	
1:A:660:LYS:HA	1:A:660:LYS:HD3	1.92	0.42	
1:A:818:LYS:HB2	1:A:819:ARG:NH1	2.34	0.42	
1:B:705:ASN:HB3 1:B:708:PHE:HB3		2.00	0.42	
1:B:942:PHE:HE2	1:B:954:PHE:HE2	1.66	0.42	
1:C:237:LYS:HE3	1:C:237:LYS:HB3	1.68	0.42	
1:C:755:TYR:HB2	1:C:804:TYR:CE2	2.55	0.42	
1:A:155:GLU:HG3	1:B:236:GLN:HG3	2.02	0.42	
1:A:233:ARG:NH2	1:D:188:ASP:OD1	2.53	0.42	
1:A:655:ILE:HA	1:A:659:PHE:CD1	2.55	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:695:ILE:HD13	1:A:699:PHE:HE2	1.83	0.42
1:B:316:ILE:HD13	1:B:316:ILE:HA	1.91	0.42
1:C:989:LYS:HE3	1:D:1001:MET:HE3	2.02	0.42
1:D:839:PHE:HA	1:D:842:LEU:CD2	2.50	0.42
1:D:962:TYR:N	1:D:962:TYR:CD1	2.88	0.42
1:A:655:ILE:O	1:A:659:PHE:HB2	2.20	0.42
1:B:414:TYR:O	1:B:657:ARG:NH2	2.43	0.42
1:B:1003:TYR:HB2	1:B:1005:ILE:HG13	2.01	0.42
1:C:262:GLU:HA	1:C:266:LEU:O	2.19	0.42
1:C:500:PHE:HA	1:C:747:ARG:HD3	2.01	0.42
1:D:250:PRO:HB3	1:D:285:ARG:HH22	1.85	0.42
1:D:744:PHE:CD2	1:D:749:LEU:HD12	2.55	0.42
2:F:22:THR:HG21	2:F:46:LYS:HE3	2.01	0.42
1:A:179:LYS:HE2	1:A:179:LYS:HB2	1.87	0.42
1:A:436:TYR:HE1	1:A:477:ASN:HD22	1.68	0.42
1:A:781:LEU:O	1:A:785:LYS:HG3	2.20	0.42
1:A:836:ASP:HB3	1:A:857:LYS:HZ2	1.84	0.42
1:A:984:LEU:HD23	1:A:1000:LEU:HD13	2.00	0.42
1:B:10:ARG:HD2	1:B:11:TYR:H	1.84	0.42
1:B:916:PHE:HD1	1:B:919:TRP:CZ3	2.37	0.42
1:C:187:GLU:O	1:C:188:ASP:HB2	2.20	0.42
1:C:742:PHE:HE1	1:C:778:PHE:HB2	8:PHE:HB2 1.85	
1:C:769:LYS:O	1:C:772:ILE:HG22	2.20	0.42
1:C:938:ASP:OD1	1:C:953:LYS:HD2	2.20	0.42
1:D:147:LYS:HG3	1:D:149:PHE:CE1	2.54	0.42
1:D:943:PHE:HZ	1:D:962:TYR:CE2	2.38	0.42
1:A:516:GLU:O	1:A:520:THR:HB	2.19	0.41
1:D:19:PHE:HA	1:D:22:LEU:HD22	2.00	0.41
1:D:151:VAL:HG12	1:D:175:ARG:HH21	1.84	0.41
1:A:875:ASP:OD1	1:A:875:ASP:N	2.52	0.41
1:B:324:TYR:OH	1:B:590:ASP:OD1	2.15	0.41
1:C:54:SER:OG	1:C:54:SER:O	2.38	0.41
1:C:146:GLY:O	1:D:471:TYR:OH	2.32	0.41
1:C:220:LEU:HD12	1:C:220:LEU:HA	1.81	0.41
1:C:352:LYS:HA	1:C:352:LYS:HD3	1.92	0.41
1:C:827:LEU:HD21	1:C:834:GLN:HB2	2.02	0.41
1:D:230:ASN:HA	1:D:233:ARG:HD2	2.01	0.41
1:D:688:LEU:HA	1:D:691:ILE:HG22	2.02	0.41
1:D:695:ILE:HG21	1:D:744:PHE:CD1	2.55	0.41
2:F:20:ILE:O	2:F:22:THR:N	2.49	0.41
2:F:101:HIS:C	2:F:101:HIS:HD1	2.23	0.41



		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (\AA)		
1:A:817:SER:OG	1:A:820:LEU:HB2	2.20	0.41	
1:A:824:THR:OG1	1:A:838:LEU:HD22	2.20	0.41	
1:B:853:LEU:HD12	1:B:853:LEU:HA	1.91	0.41	
2:E:68:SER:OG	2:E:73:LEU:HD21	2.20	0.41	
1:C:117:ILE:HD13	1:C:120:LYS:HD2 2.01		0.41	
1:D:514:ARG:O	1:D:518:GLU:HG2	2.20	0.41	
1:A:23:ASP:OD1	1:A:24:ASN:N	2.53	0.41	
1:A:359:ARG:HA	1:A:359:ARG:HD2	1.92	0.41	
1:A:480:ARG:HB3	1:A:601:TRP:HD1	1.84	0.41	
1:A:741:LEU:HA	1:A:741:LEU:HD13	1.93	0.41	
1:A:984:LEU:HD23	1:A:1000:LEU:HB2	2.01	0.41	
1:C:236:GLN:HG2	1:C:239:SER:HB3	2.02	0.41	
1:C:338:TYR:CZ	1:C:357:MET:HB2	2.55	0.41	
1:D:287:SER:O	1:D:291:ASP:OD1	2.37	0.41	
1:D:827:LEU:HD23	1:D:831:LYS:HE3	2.01	0.41	
1:A:157:ASP:OD2	1:A:175:ARG:NH2	2.53	0.41	
1:A:247:ARG:CZ	1:A:249:ASP:HB2	2.50	0.41	
1:A:682:GLU:H	1:A:682:GLU:HG3	1.73	0.41	
1:A:802:ARG:HH22	1:A:870:ARG:HE	1.68	0.41	
2:E:14:LEU:HD13	2:E:25:TRP:CD2	2.56	0.41	
1:D:973:ASN:C	1:D:975:HIS:H	2.24	0.41	
1:A:407:ILE:HD13	1:A:589:TYR:CD2	2.56	0.41	
1:A:831:LYS:H	1:A:831:LYS:HG2	1.57	0.41	
1:B:492:PHE:CE2	1:B:506:PRO:HG3	2.56	0.41	
1:B:978:HIS:O	1:B:981:ILE:HG22	2.20	0.41	
1:C:35:GLU:HG3	1:C:35:GLU:H	1.69	0.41	
1:C:412:LEU:HB2	1:C:441:PHE:CZ	2.56	0.41	
1:D:17:GLU:C	1:D:17:GLU:OE1	2.58	0.41	
1:D:256:GLU:O	1:D:259:ILE:HG12	2.21	0.41	
1:D:295:GLU:HB3	1:D:300:LYS:HB2	2.02	0.41	
1:A:500:PHE:HA	1:A:747:ARG:HD3	2.03	0.41	
1:A:677:ARG:HE	1:A:677:ARG:HB2	1.71	0.41	
1:A:967:LEU:HB3	1:A:1005:ILE:HD11	2.03	0.41	
1:A:985:LYS:HA	1:B:1001:MET:CE	2.51	0.41	
1:B:139:ASP:OD2	1:B:169:LYS:NZ	2.52	0.41	
1:B:432:ILE:HD12	1:B:432:ILE:HA	1.89	0.41	
1:C:749:LEU:HA	1:C:749:LEU:HD12	1.86	0.41	
1:D:448:TRP:CD1	1:D:481:ILE:HD11	2.56	0.41	
1:A:387:PHE:O	1:A:391:ASN:HB2	2.21	0.41	
1:A:981:ILE:HD13	1:A:981:ILE:HA	1.93	0.41	
1:C:842:LEU:HD13	1:C:853:LEU:HD23	2.03	0.41	



	lo uo pugo	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:155:GLU:OE2	1:A:155:GLU:HA	2.20	0.41	
1:A:660:LYS:O	1:A:664:ILE:HG13	2.20	0.41	
1:A:947:GLU:H	1:A:947:GLU:CD	2.23	0.41	
1:B:28:GLU:O	1:B:32:GLU:HG3	2.21	0.41	
1:B:122:LEU:HD13	1:B:122:LEU:HA	1.87	0.41	
1:B:647:MET:HE1	1:B:722:PHE:HE2	1.86	0.41	
1:B:970:ILE:HG23	1:B:976:MET:SD	2.60	0.41	
1:C:42:LEU:O	1:C:127:ALA:N	2.50	0.41	
1:C:319:LEU:HD11	1:C:333:VAL:HG21	2.02	0.41	
1:C:817:SER:OG	1:C:820:LEU:HB2	2.21	0.41	
1:D:377:GLN:N	1:D:377:GLN:OE1	2.54	0.41	
1:A:502:ARG:NH1	1:A:504:TYR:HA	2.36	0.41	
1:A:981:ILE:HG12	1:A:1005:ILE:O	2.21	0.41	
1:B:22:LEU:HD11	1:B:274:LEU:HD22	2.02	0.41	
1:B:687:TYR:CZ	1:B:691:ILE:HD11	2.55	0.41	
1:C:416:GLY:HA2	1:C:418:TYR:HE1	1.85	0.41	
1:C:987:ARG:HA	1:C:987:ARG:NE	2.36	0.41	
1:D:738:LYS:HB2	1:D:738:LYS:HE2	1.71	0.41	
1:A:828:THR:O	1:A:835:ILE:HD11	2.21	0.40	
1:B:886:ILE:HD13	1:B:886:ILE:HA 1.90		0.40	
1:B:957:SER:HB3	2:E:21:ASN:ND2	2.37	0.40	
2:E:56:LYS:HD2	2:E:56:LYS:HA	1.93	0.40	
1:C:361:PHE:HD2	1:C:396:MET:SD	2.45	0.40	
1:A:472:TYR:HD1	1:A:531:MET:HE3	1.86	0.40	
1:A:491:GLN:O	1:A:496:GLY:N	2.55	0.40	
1:A:595:LEU:HB3	1:A:603:VAL:HG12	2.03	0.40	
1:B:220:LEU:HD23	1:B:220:LEU:HA	1.89	0.40	
1:B:247:ARG:CZ	1:B:249:ASP:HB2	2.51	0.40	
1:B:281:ASP:HB3	1:B:284:GLU:OE1	2.22	0.40	
1:C:953:LYS:HB2	1:C:953:LYS:HE2	1.81	0.40	
1:A:319:LEU:HD11	1:A:333:VAL:HG21	2.03	0.40	
1:A:1003:TYR:HB2	1:A:1005:ILE:CG1	2.51	0.40	
1:D:602:SER:HA	1:D:605:PHE:CD2	2.56	0.40	
1:D:649:TYR:HE1	1:D:687:TYR:HB2	1.87	0.40	
1:D:924:GLU:OE1 2:F:57:CYS:HA		2.21	0.40	
1:A:376:LYS:O	1:A:379:GLU:HG2	2.21	0.40	
1:A:448:TRP:HA	1:A:451:SER:OG	2.22	0.40	
1:A:724:LYS:HB2	1:A:760:ARG:HB3	2.02	0.40	
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.85	0.40	
1:B:140:THR:HG22	1:B:144:LYS:HE3	2.03	0.40	
1:B:827:LEU:HA	1:B:827:LEU:HD23	1.90	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:700:SER:HB2	1:D:743:TYR:CE1	2.57	0.40
1:D:869:ILE:HD11	2:F:57:CYS:SG	2.62	0.40
1:A:920:TYR:CD1	1:A:930:MET:HE2	2.56	0.40
1:B:624:GLU:O	1:B:628:THR:HG23	2.21	0.40
1:B:914:SER:O	1:B:918:ILE:HG13	2.21	0.40
1:C:229:LEU:HD21	1:C:266:LEU:HG	2.04	0.40
1:C:846:SER:O	1:C:850:LYS:HG2	2.21	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	entiles
1	А	941/1005~(94%)	925~(98%)	16 (2%)	0	100	100
1	В	939/1005~(93%)	921 (98%)	18 (2%)	0	100	100
1	С	940/1005~(94%)	928 (99%)	12 (1%)	0	100	100
1	D	939/1005~(93%)	921 (98%)	18 (2%)	0	100	100
2	Е	114/146~(78%)	111 (97%)	3(3%)	0	100	100
2	F	114/146~(78%)	108 (95%)	6 (5%)	0	100	100
All	All	3987/4312~(92%)	3914 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent 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



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	878/923~(95%)	821 (94%)	57~(6%)	17	22
1	В	877/923~(95%)	820 (94%)	57~(6%)	17	22
1	С	877/923~(95%)	819~(93%)	58 (7%)	16	21
1	D	877/923~(95%)	821 (94%)	56 (6%)	17	22
2	Ε	111/131~(85%)	99~(89%)	12 (11%)	6	7
2	F	111/131~(85%)	102 (92%)	9 (8%)	11	15
All	All	3731/3954~(94%)	3482 (93%)	249 (7%)	20	21

analysed, and the total number of residues.

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	14	LYS
1	А	19	PHE
1	А	32	GLU
1	А	45	PHE
1	А	73	SER
1	А	82	ASP
1	А	95	LYS
1	А	107	PHE
1	А	134	TYR
1	А	135	ASP
1	А	145	ARG
1	А	281	ASP
1	А	284	GLU
1	А	303	THR
1	А	304	LYS
1	А	306	ASP
1	А	402	THR
1	А	404	ASN
1	А	456	SER
1	А	497	LEU
1	А	508	THR
1	A	525	ASP
1	А	533	PHE
1	А	540	LYS
1	A	557	LYS
1	A	579	SER
1	A	581	ASP
1	А	590	ASP



Mol	Chain	Res	Type
1	А	629	ARG
1	А	646	PHE
1	А	662	ASP
1	А	674	ASP
1	А	677	ARG
1	А	710	THR
1	А	714	SER
1	А	738	LYS
1	А	757	TRP
1	А	763	LYS
1	А	765	ASN
1	А	766	GLU
1	А	769	LYS
1	А	784	GLU
1	А	809	LYS
1	А	814	ASN
1	А	819	ARG
1	А	825	LEU
1	А	834	GLN
1	А	875	ASP
1	А	913	MET
1	А	920	TYR
1	А	930	MET
1	А	954	PHE
1	А	957	SER
1	А	964	ASP
1	А	976	MET
1	А	978	HIS
1	А	995	ARG
1	В	10	ARG
1	В	25	ASN
1	В	45	PHE
1	В	86	ARG
1	В	115	ASN
1	В	134	TYR
1	В	138	ILE
1	В	147	LYS
1	В	186	LYS
1	В	222	ASP
1	В	226	ASN
1	В	227	MET
1	В	236	GLN



Mol	Chain	Res	Type
1	В	239	SER
1	В	249	ASP
1	В	281	ASP
1	В	304	LYS
1	В	328	ILE
1	В	389	GLU
1	В	398	LYS
1	В	431	SER
1	В	463	ILE
1	В	467	ASN
1	В	484	SER
1	В	502	ARG
1	В	505	LYS
1	В	509	ASP
1	В	526	ASP
1	В	540	LYS
1	В	553	ASP
1	В	590	ASP
1	В	615	SER
1	В	633	GLU
1	В	665	LYS
1	В	669	ARG
1	В	671	CYS
1	В	674	ASP
1	В	714	SER
1	В	722	PHE
1	В	744	PHE
1	В	748	ASP
1	В	750	ASP
1	В	754	ARG
1	В	765	ASN
1	В	802	ARG
1	В	810	HIS
1	В	811	PHE
1	В	839	PHE
1	В	863	ASN
1	В	892	ARG
1	В	927	ASN
1	В	933	PHE
1	В	942	PHE
1	В	969	LYS
1	В	976	MET



Mol	Chain	Res	Type
1	В	1000	LEU
1	В	1002	ASN
2	Е	11	THR
2	Е	18	SER
2	Е	22	THR
2	Е	36	SER
2	Е	43	TYR
2	Е	49	ASN
2	Е	52	ARG
2	Е	72	ARG
2	Е	77	ASN
2	Е	88	HIS
2	Е	110	PHE
2	E	115	GLU
1	С	21	MET
1	C	45	PHE
1	С	82	ASP
1	С	98	MET
1	С	107	PHE
1	С	134	TYR
1	С	140	THR
1	С	237	LYS
1	С	298	GLU
1	С	303	THR
1	С	306	ASP
1	С	310	ASP
1	С	342	VAL
1	С	375	LYS
1	C	408	GLU
1	С	419	ASP
1	С	421	MET
1	С	491	GLN
1	С	497	LEU
1	C	516	GLU
1	С	533	PHE
1	С	554	ASP
1	С	561	LEU
1	С	573	SER
1	С	578	MET
1	С	588	LEU
1	C	590	ASP
1	С	593	ARG



Mol	Chain	Res	Type
1	С	624	GLU
1	С	667	LEU
1	С	674	ASP
1	С	708	PHE
1	С	744	PHE
1	С	750	ASP
1	С	757	TRP
1	С	763	LYS
1	С	804	TYR
1	С	818	LYS
1	С	859	VAL
1	С	865	LEU
1	С	881	HIS
1	С	912	TYR
1	С	913	MET
1	С	928	SER
1	С	930	MET
1	С	939	GLN
1	С	940	TYR
1	С	941	ASP
1	С	952	LYS
1	С	961	ASN
1	С	963	ASN
1	С	974	LYS
1	С	976	MET
1	С	977	LYS
1	С	982	GLU
1	С	987	ARG
1	С	1001	MET
1	С	1004	PHE
1	D	17	GLU
1	D	21	MET
1	D	23	ASP
1	D	45	PHE
1	D	69	GLU
1	D	81	SER
1	D	107	PHE
1	D	134	TYR
1	D	147	LYS
1	D	160	ASN
1	D	183	VAL
1	D	233	ARG



Mol	Chain	Res	Type
1	D	249	ASP
1	D	267	ARG
1	D	285	ARG
1	D	300	LYS
1	D	342	VAL
1	D	348	ARG
1	D	374	SER
1	D	375	LYS
1	D	389	GLU
1	D	395	CYS
1	D	398	LYS
1	D	399	ASP
1	D	423	LYS
1	D	484	SER
1	D	505	LYS
1	D	517	ARG
1	D	526	ASP
1	D	540	LYS
1	D	548	ASN
1	D	590	ASP
1	D	671	CYS
1	D	672	SER
1	D	680	GLU
1	D	685	GLU
1	D	710	THR
1	D	714	SER
1	D	722	PHE
1	D	738	LYS
1	D	740	LEU
1	D	744	PHE
1	D	747	ARG
1	D	755	TYR
1	D	781	LEU
1	D	795	SER
1	D	848	ASN
1	D	857	LYS
1	D	886	ILE
1	D	932	GLU
1	D	933	PHE
1	D	953	LYS
1	D	957	SER
1	D	975	HIS



Mol	Chain	\mathbf{Res}	Type
1	D	978	HIS
1	D	994	LYS
2	F	39	LEU
2	F	44	PHE
2	F	52	ARG
2	F	71	LYS
2	F	72	ARG
2	F	101	HIS
2	F	108	SER
2	F	114	LYS
2	F	115	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	115	ASN
1	А	765	ASN
1	В	202	ASN
1	В	832	GLN
2	Е	49	ASN
2	Е	123	HIS
1	С	89	GLN
1	С	196	ASN
1	С	297	GLN
1	С	457	ASN
1	С	523	ASN
1	С	711	GLN
1	С	979	HIS
1	С	1002	ASN
1	D	927	ASN
2	F	88	HIS

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)

There are no ligands in this entry.

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-37924. 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



6.2.2 Raw map



X Index: 280

Y Index: 280



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: 295



Y Index: 265



Z Index: 257

6.3.2 Raw map



X Index: 295

Y Index: 265



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

A mask typically either:

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

$emd_{37924}_{msk}_{1.map}$ (i) 6.6.1





7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 153 $\rm nm^3;$ this corresponds to an approximate mass of 138 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 0.391 ${\rm \AA^{-1}}$



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 0.391 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\frac{1}{2}$	Estim	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	2.56	-	-	
Author-provided FSC curve	3.65	7.80	3.80	
Unmasked-calculated*	3.64	7.74	3.78	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 2.56 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 2.56 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37924 and PDB model 8WYD. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.4 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 (0.4).



9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5570	0.3520
А	0.8330	0.5110
В	0.8510	0.5300
С	0.2890	0.1860
D	0.3050	0.2140
Е	0.6880	0.4290
F	0.0020	0.0130

