

Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 12:39 PM EDT

PDB ID	:	8FUF
Title	:	Crystal structure of human O-GlcNAc transferase (OGT) in complex with an
		exosite-binding peptide (ZNF831) and UDP-GlcNAc
Authors	:	Xie, J.; Jiang, J.
Deposited on	:	2023-01-17
Resolution	:	3.69 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 3.69 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	Similar resolution							
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$							
R _{free}	130704	1049 (3.88-3.52)							
Clashscore	141614	1027 (3.86-3.54)							
Ramachandran outliers	138981	1069 (3.88-3.52)							
Sidechain outliers	138945	1065 (3.88-3.52)							
RSRZ outliers	127900	1578(3.90-3.50)							

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain												
1	А	723	.% 5 6%	40%	·										
1	С	723	% 5 7%	38%	•										
1	Е	723	2% 51%	44%	·										
1	G	723	.% 51%	44%											
2	В	13	46% 38%												



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Mol	Chain	Length	Quality of chain												
0	П	12	224	2001	150/										
	D	10	23%	62%	15%										
			15%												
2	F	13	31%	54%	15%										
			8%												
2	Н	13	31%	54%	15%										



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22524 atoms, of which 32 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltran sferase 110 kDa subunit.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
1	Δ	605	Total	С	Ν	Ο	S	5	0	0
	Л	095	5492	3485	960	1010	37	5	0	0
1	С	605	Total	С	Ν	Ο	S	5	0	0
	U	095	5492	3485	960	1010	37	5	0	0
1	F	605	Total	С	Ν	Ο	S	5	0	0
	Ľ	095	5492	5492 3485 960 1010 37		5	0	0		
1	C	605	Total	С	Ν	Ο	S	5	0	0
	G	095	5492	3485	960	1010	37	0	U	U

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference					
А	309	GLY	-	expression tag	UNP O15294					
А	310	PRO	-	expression tag	UNP O15294					
А	311	GLY	-	expression tag	UNP O15294					
А	312	SER	-	expression tag	UNP O15294					
С	309	GLY	-	expression tag	UNP O15294					
С	310	PRO	-	expression tag	UNP O15294					
С	311	GLY	-	expression tag	UNP O15294					
С	312	SER	-	expression tag	UNP O15294					
E	309	GLY	-	expression tag	UNP O15294					
Е	310	PRO	-	expression tag	UNP O15294					
E	311	GLY	-	expression tag	UNP O15294					
E	312	SER	-	expression tag	UNP O15294					
G	309	GLY	-	expression tag	UNP O15294					
G	310	PRO	-	expression tag	UNP O15294					
G	311	GLY	-	expression tag	UNP O15294					
G	312	SER	-	expression tag	UNP 015294					

• Molecule 2 is a protein called Zinc finger protein 831.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	В	11	Total	С	Η	Ν	0	0	0	0
	D	11	100	64	8	15	13	0	0	0
0	л	11	Total	С	Η	Ν	0	0	0	0
	D	11	100	64	8	15	13	0	0	0
0	F	11	Total	С	Η	Ν	0	0	0	0
	Г	11	100	64	8	15	13	0	0	0
9	и	11	Total	С	Н	Ν	0	0	0	0
	11		100	64	8	15	13	0		0

• Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms	ZeroOcc	AltConf		
2	Δ	1	Total	С	Ν	Ο	Р	0	0
0	A	1	39	17	3	17	2	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0
0	U	1	39	17	3	17	2	0	0
2	F	1	Total	С	Ν	Ο	Р	0	0
0	Ľ	1	39	17	3	17	2	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0
3	G	1	39	17	3	17	2	0	U



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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

 \bullet Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



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Chain C: 57% 38% •





 \bullet Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

Cha	air	1 I	E:	2%	,								51	L%																	44	1%								•					
GLY PRO	SER	CYS	T315	H316	A317 D318	S319	L320	N321	N322	L323	N325	1326	K327	R328	13 <mark>33</mark>	-	V337	K338 1 2 2 0	Y340	R341	K342	A343 1344	E345	V346	F347	P348 F349	F350	A351	A352	H-CO-CH	N356	L357	A350 S359	<mark>V360</mark>	L361	0362	u,364 0364	G365	K366	L367 D368	E369	A370	L371 M372	H373	Y374
K375 E376 A 277	A377 1378	R379	1380	F384	A387	Y388	<mark>5389</mark>	N390	M391	1392 N303		E397	M398	<mark>1</mark> 399	L405	-	Y408	1.409 D.110		I412	Q413	1414 N215		F418	A419	D420 A421	H422		L425	8420 S427	1428	H429	S432	-	E437	A438	A440	S441	Y442	A445	L446	-	K449	F452	P453
D454 A455 VAE6	14.50 C457	N458	L409	L463	V466		W469	T470	D471	FA74	R475	M476		L479 V480	S481	I482	V483	A484	E488	K489	N490	R491 1492	P493	S494		P497 H498		M501		S506	H507	G508	R510	K511	A512	1513 Ac14	E515	R516	H517	1.5.20		D523	N526		Y533
P536	D538	L539	K540 L541		R545 1.546	R547	V548		V551	2002 2553	D554	F555		H558 P559		M564	Q565	5566 TE67		P573		F576	C580	Y581	A582	L583	N590	F591	R592	K594	V595	M596	F602	-	A614	ne10	eTou	G622	, , , , , ,	T626	M629	N630	G631 Y632	T633	•
R637	п040	R644	C PO4	0649	A650 M651	W652	L653	G654	Y655	TEER	1000 S659	-	Y666	1667 1668	1669 T669	-	E672	NG78	A679	E680	Q681	Y682	E684	K685	L686	A687 V688	M689	P690	1000	H698		K706	K708	-		D712 E713	K714	S715	ASN	GLY HTS	1719	Y720	R723		L726





 \bullet Molecule 1: UDP-N-acetyl
glucosamine--peptide N-acetylglucosaminyl
transferase 110 kDa subunit



• Molecule 2: Zinc finger protein 831



Chain B:	46%	38%	15%
ASN A936 F937 8938 1939 1948 L943 L946	CL2		
• Molecule 2:	Zinc finger protein 8	331	
Chain D:	23%	62%	15%
ASN A936 F937 5938 5938 7941 L943 L943 L943 L943	1246 GLN GLN		
• Molecule 2:	Zinc finger protein 8	331	
1	5%		
Chain F:	31%	54%	15%
ASN A936 F937 F938 F938 F941 L943 L943 L943 C944	9 966d		
• Molecule 2:	Zinc finger protein 8	331	
8%			
Chain H:	31%	54%	15%
ASN A936 5937 5938 5938 2939 7941 1942 1943 1944	c <mark>1946 d</mark> C TIN		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants	274.01Å 274.01Å 143.08Å	Deneriten
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\mathbf{\hat{\lambda}})$	53.06 - 3.69	Depositor
Resolution (A)	53.06 - 3.69	EDS
% Data completeness	99.1 (53.06-3.69)	Depositor
(in resolution range)	91.6(53.06-3.69)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.43 (at 3.67 Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.198 , 0.242	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.199 , 0.240	DCC
R_{free} test set	1989 reflections (3.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	111.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.35, 115.1	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22524	wwPDB-VP
Average B, all atoms $(Å^2)$	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: UD1

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

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/5618	0.44	0/7619
1	С	0.24	0/5618	0.44	0/7619
1	Е	0.24	0/5618	0.43	0/7619
1	G	0.24	0/5618	0.44	0/7619
2	В	0.26	0/95	0.55	0/128
2	D	0.23	0/95	0.58	0/128
2	F	0.24	0/95	0.53	0/128
2	Н	0.26	0/95	0.55	0/128
All	All	0.24	0/22852	0.44	0/30988

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5492	0	5464	273	0
1	С	5492	0	5464	252	0
1	Е	5492	0	5464	305	0
1	G	5492	0	5464	291	0
2	В	92	8	100	10	0



	J	1	1 5			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	92	8	100	10	0
2	F	92	8	100	19	0
2	Н	92	8	100	16	0
3	А	39	0	25	6	0
3	С	39	0	25	3	0
3	Ε	39	0	25	2	0
3	G	39	0	25	11	0
All	All	22492	32	22356	1138	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 25.

All (1138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:712:ASP:HA	1:E:719:ILE:HD11	1.32	1.08
1:C:388:TYR:HA	1:C:391:MET:HB3	1.37	1.06
1:A:854:ILE:HD11	1:A:967:GLU:HA	1.33	1.05
1:E:798:LEU:HD11	1:E:824:GLN:HB3	1.38	1.02
1:E:777:ILE:HG12	2:F:943:LEU:HD23	1.44	0.97
1:E:631:GLY:HA3	1:E:655:TYR:HB2	1.45	0.97
1:E:826:GLY:HA3	2:F:940:LYS:HE3	1.47	0.96
1:E:426:ALA:HB2	1:E:441:SER:HB2	1.47	0.95
1:G:317:ALA:HB1	1:G:343:ALA:HB1	1.50	0.92
1:A:798:LEU:HG	1:A:824:GLN:HE21	1.31	0.92
1:E:842:LYS:HB2	1:E:914:THR:HG21	1.53	0.91
1:G:324:ALA:HB2	1:G:339:LEU:HB2	1.54	0.90
1:E:374:TYR:HB3	1:E:391:MET:HE2	1.55	0.88
1:A:327:LYS:HD2	1:A:332:ASN:HD22	1.39	0.87
1:C:605:LEU:HA	1:C:608:ILE:HD12	1.57	0.87
1:A:726:LEU:HD22	1:A:819:VAL:HG22	1.58	0.85
1:C:839:GLN:HG2	1:C:868:PHE:CE2	2.11	0.85
1:A:362:GLN:HE22	1:A:370:ALA:HB1	1.42	0.85
2:D:938:SER:OG	2:D:939:PRO:HD2	1.77	0.85
1:A:426:ALA:HB2	1:A:441:SER:HB2	1.60	0.84
1:C:396:LYS:HE2	1:C:428:ILE:HG22	1.58	0.84
1:C:673:THR:HG21	1:C:693:PHE:HE1	1.44	0.83
1:C:570:MET:SD	1:C:999:THR:OG1	2.35	0.83
1:G:336:ALA:HA	1:G:339:LEU:HD13	1.61	0.83
1:A:358:ALA:HB2	1:A:373:HIS:HB2	1.60	0.82
1:A:335:GLU:HB3	1:A:338:ARG:HH11	1.41	0.82



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:552:SER:HB2	1:E:629:MET:HB2	1.61	0.82
1:G:559:PRO:HB2	3:G:1201:UD1:H6'2	1.60	0.81
1:E:333:ILE:HD11	1:E:360:VAL:HB	1.63	0.80
2:H:942:LEU:H	2:H:942:LEU:HD23	1.45	0.79
1:E:405:LEU:O	1:E:409:THR:HG23	1.83	0.79
1:E:323:LEU:O	1:E:326:ILE:HG22	1.83	0.79
1:C:644:ARG:HA	1:C:649:GLN:HE22	1.47	0.79
1:E:713:PHE:HE1	1:E:720:TYR:H	1.29	0.79
1:A:675:PRO:O	1:A:678:VAL:HG12	1.82	0.78
1:A:366:LYS:HB3	1:A:369:GLU:HB2	1.65	0.78
1:E:553:SER:HB3	1:E:583:LEU:HB2	1.64	0.78
1:E:947:ALA:O	1:E:951:THR:HG23	1.83	0.78
1:C:552:SER:HB2	1:C:629:MET:HB2	1.66	0.78
1:E:933:MET:SD	1:E:950:LEU:HD21	2.24	0.78
1:G:337:VAL:O	1:G:341:ARG:HG2	1.83	0.78
2:D:942:LEU:HD23	2:D:942:LEU:H	1.49	0.78
1:E:325:ASN:O	1:E:328:ARG:HG2	1.84	0.77
1:C:836:ASN:HD21	1:C:914:THR:HG23	1.49	0.77
2:F:938:SER:HB2	2:F:939:PRO:HD2	1.66	0.77
2:F:945:LEU:O	2:F:945:LEU:HD12	1.84	0.77
1:C:378:ILE:HD12	1:C:388:TYR:HD2	1.50	0.76
1:A:395:LEU:HG	1:A:400:ASP:HB3	1.66	0.76
1:E:327:LYS:HE3	1:E:327:LYS:HA	1.66	0.76
1:G:335:GLU:O	1:G:339:LEU:HD12	1.86	0.76
1:A:322:ASN:O	1:A:326:ILE:HG12	1.86	0.76
1:A:823:SER:CB	2:B:943:LEU:HD11	2.16	0.75
1:E:805:ASN:O	1:E:809:THR:HG23	1.85	0.75
1:G:839:GLN:HB2	1:G:841:TYR:CD1	2.22	0.75
1:E:323:LEU:HB3	1:E:339:LEU:HD21	1.68	0.75
1:E:777:ILE:HG23	2:F:943:LEU:HB3	1.68	0.75
1:G:512:ALA:O	1:G:516:ARG:HG2	1.86	0.75
1:A:564:MET:HA	1:A:567:ILE:HD13	1.69	0.75
1:A:689:MET:HE3	1:A:690:PRO:HD2	1.68	0.75
1:A:780:ILE:O	2:B:939:PRO:HD3	1.86	0.75
1:A:361:LEU:CD1	1:A:369:GLU:HG2	2.16	0.74
1:C:408:TYR:O	1:C:412:ILE:HD12	1.87	0.74
1:G:823:SER:HA	2:H:941:TYR:CE2	2.23	0.74
1:E:900:GLU:O	1:E:904:ARG:HG2	1.86	0.74
1:A:484:ALA:O	1:A:488:GLU:HG2	1.88	0.73
1:E:854:ILE:HD11	1:E:967:GLU:HA	1.71	0.73
1:E:405:LEU:HD11	1:G:414:ILE:HG12	1.71	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:724:ILE:HG23	1:C:821:THR:HG22	1.70	0.72
1:G:687:ALA:HB1	1:G:1009:LEU:HD21	1.71	0.72
1:A:327:LYS:HB3	1:A:336:ALA:HB2	1.70	0.72
1:A:521:CYS:O	1:A:525:ILE:HG23	1.89	0.72
1:C:371:LEU:HD11	1:C:395:LEU:HD21	1.72	0.72
1:A:644:ARG:HH21	1:A:663:PHE:HA	1.54	0.72
1:A:359:SER:HA	1:A:362:GLN:HG2	1.69	0.72
1:A:473:ASP:O	1:A:477:LYS:HG2	1.89	0.72
1:C:405:LEU:HD13	1:C:428:ILE:CD1	2.19	0.72
1:G:366:LYS:HG3	1:G:369:GLU:CD	2.09	0.72
1:C:366:LYS:HG3	1:C:368:GLN:O	1.90	0.72
1:A:1003:THR:O	1:A:1007:GLU:HG3	1.89	0.72
1:C:426:ALA:HB2	1:C:441:SER:HB2	1.72	0.72
1:G:918:ASN:HD22	1:G:946:ALA:H	1.37	0.72
1:E:678:VAL:HG21	1:E:681:GLN:NE2	2.05	0.71
1:G:426:ALA:HB2	1:G:441:SER:HB2	1.71	0.71
1:C:673:THR:HG21	1:C:693:PHE:CE1	2.25	0.71
1:A:525:ILE:HD12	1:A:643:LEU:HD12	1.71	0.71
1:G:405:LEU:O	1:G:409:THR:HG23	1.88	0.71
1:E:914:THR:HG22	1:E:917:CYS:H	1.56	0.71
1:G:320:LEU:HD12	1:G:343:ALA:HA	1.72	0.71
1:G:909:ASP:HA	1:G:984:ARG:NH2	2.05	0.71
1:E:774:GLU:OE2	2:F:945:LEU:HD13	1.90	0.71
1:A:583:LEU:HD22	1:A:637:ARG:HD3	1.72	0.71
1:A:854:ILE:HD12	1:A:970:ALA:HB3	1.73	0.71
1:C:873:GLU:HG3	1:C:892:PHE:CD2	2.25	0.70
1:A:800:THR:HA	1:A:803:ILE:HG22	1.73	0.70
1:C:409:THR:O	1:C:413:GLN:HG3	1.91	0.70
1:G:317:ALA:HB1	1:G:343:ALA:CB	2.20	0.70
1:C:697:ASP:OD2	1:C:700:ASN:HB3	1.91	0.70
1:C:805:ASN:O	1:C:809:THR:HG23	1.92	0.70
1:G:320:LEU:HD13	1:G:342:LYS:HG3	1.73	0.70
1:E:357:LEU:O	1:E:361:LEU:HG	1.92	0.70
1:E:371:LEU:HD12	1:E:372:MET:N	2.07	0.69
1:G:831:ALA:HB1	1:G:860:ASN:O	1.92	0.69
1:A:361:LEU:HD11	1:A:369:GLU:HG2	1.75	0.69
1:G:462:CYS:HA	1:G:465:ILE:HD12	1.73	0.69
1:A:841:TYR:OH	3:A:1201:UD1:H8'1	1.92	0.69
1:E:426:ALA:HB2	1:E:441:SER:CB	2.20	0.69
1:A:442:TYR:O	1:A:446:LEU:HG	1.92	0.69
1:E:839:GLN:HA	1:E:868:PHE:HD2	1.55	0.69



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:833:VAL:HG21	1:G:908:ALA:HA	1.74	0.69
1:C:418:PHE:CE2	1:C:420:ASP:HB2	2.26	0.69
1:E:800:THR:HA	1:E:803:ILE:HD12	1.73	0.69
1:E:357:LEU:HD23	1:E:373:HIS:NE2	2.08	0.69
1:A:852:ALA:O	1:A:856:LYS:HG3	1.92	0.69
1:C:590:ASN:HD22	1:C:811:GLU:HB3	1.58	0.69
1:E:366:LYS:HZ2	1:E:368:GLN:HB2	1.57	0.69
1:E:852:ALA:O	1:E:856:LYS:HG2	1.93	0.69
1:G:366:LYS:HG3	1:G:369:GLU:OE1	1.92	0.69
1:G:476:MET:HE2	1:G:504:PRO:HD2	1.74	0.69
1:A:418:PHE:CE1	1:A:420:ASP:HB2	2.28	0.69
1:C:822:ARG:HG3	1:C:907:LEU:HD22	1.75	0.69
1:E:806:LYS:CD	1:E:811:GLU:HB2	2.23	0.69
1:C:652:TRP:NE1	1:C:653:LEU:HD13	2.07	0.69
1:G:333:ILE:O	1:G:337:VAL:HG23	1.92	0.69
1:G:591:PHE:O	1:G:595:VAL:HG23	1.92	0.69
1:C:433:GLY:O	1:C:435:ILE:HD12	1.92	0.68
1:C:388:TYR:O	1:C:407:CYS:HB3	1.93	0.68
1:A:687:ALA:HB1	1:A:1009:LEU:HD21	1.74	0.68
1:G:357:LEU:O	1:G:360:VAL:HG12	1.93	0.68
1:G:562:HIS:CE1	1:G:898:LYS:HE3	2.29	0.68
1:C:367:LEU:HD13	1:C:397:GLU:HB2	1.76	0.68
1:G:1003:THR:O	1:G:1007:GLU:HG3	1.93	0.68
1:C:650:ALA:HB2	1:C:666:TYR:HB2	1.75	0.68
1:E:489:LYS:HB2	1:E:491:ARG:HG3	1.74	0.68
1:G:408:TYR:CE2	1:G:424:ASN:HB3	2.28	0.68
1:A:690:PRO:HG2	1:A:1005:GLU:CD	2.14	0.68
2:B:938:SER:HB2	2:B:939:PRO:HD2	1.74	0.68
1:G:586:ASP:HA	1:G:592:ARG:HD3	1.76	0.68
1:C:332:ASN:ND2	1:C:335:GLU:HB3	2.08	0.67
1:E:826:GLY:HA3	2:F:940:LYS:CE	2.23	0.67
1:E:323:LEU:CB	1:E:339:LEU:HD21	2.24	0.67
1:G:781:ASN:HA	2:H:939:PRO:HG2	1.75	0.67
1:G:833:VAL:CG2	1:G:908:ALA:HA	2.24	0.67
1:G:852:ALA:O	1:G:856:LYS:HG3	1.95	0.67
1:A:426:ALA:HB2	1:A:441:SER:CB	2.24	0.67
1:A:827:LEU:HD11	1:A:864:TRP:CE3	2.30	0.67
1:A:357:LEU:HD13	1:A:373:HIS:CE1	2.28	0.67
1:G:461:HIS:O	1:G:465:ILE:HG13	1.94	0.67
1:C:349:GLU:HA	1:C:380:ILE:HD13	1.77	0.67
1:E:822:ARG:HD3	1:E:827:LEU:HB2	1.75	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:836:ASN:ND2	1:C:914:THR:HG23	2.10	0.67
1:C:1012:GLN:HB3	1:C:1026:MET:CE	2.24	0.67
1:E:360:VAL:O	1:E:364:GLN:HG2	1.95	0.67
1:A:726:LEU:CD2	1:A:819:VAL:HG22	2.26	0.67
1:E:669:THR:HG21	1:E:686:LEU:HD22	1.76	0.66
1:A:854:ILE:HD11	1:A:967:GLU:CA	2.19	0.66
1:C:853:ASN:O	1:C:857:ARG:HG3	1.95	0.66
1:E:344:LEU:CD2	1:E:353:ALA:HB1	2.26	0.66
1:G:671:GLN:O	1:G:672:GLU:HB3	1.95	0.66
1:C:374:TYR:HB3	1:C:391:MET:CE	2.26	0.66
1:C:669:THR:HA	1:C:693:PHE:CD1	2.30	0.66
1:C:1003:THR:O	1:C:1007:GLU:HG3	1.95	0.66
1:C:324:ALA:HB2	1:C:339:LEU:CB	2.26	0.66
1:G:327:LYS:HE2	1:G:335:GLU:HG2	1.78	0.66
1:E:714:LYS:O	1:E:714:LYS:HG2	1.95	0.66
1:G:576:PHE:CZ	1:G:1007:GLU:HB3	2.30	0.66
1:C:1001:GLN:O	1:C:1005:GLU:HG3	1.95	0.66
1:G:839:GLN:HG2	1:G:868:PHE:CE2	2.31	0.66
1:E:333:ILE:O	1:E:337:VAL:HG23	1.95	0.66
1:G:692:THR:HG21	1:G:996:LEU:HD13	1.78	0.66
1:A:923:GLY:O	1:A:927:LEU:HG	1.97	0.65
1:C:374:TYR:O	1:C:378:ILE:HG12	1.95	0.65
1:E:342:LYS:O	1:E:346:VAL:HG23	1.96	0.65
1:G:725:VAL:HG12	1:G:820:THR:HB	1.77	0.65
1:A:828:PRO:HG2	1:A:831:ALA:HB3	1.77	0.65
1:C:644:ARG:HA	1:C:649:GLN:NE2	2.12	0.65
1:E:545:ARG:HD3	1:E:573:PRO:O	1.96	0.65
1:G:963:ARG:H	1:G:963:ARG:HD3	1.62	0.65
1:C:376:GLU:O	1:C:380:ILE:HG13	1.96	0.65
1:G:777:ILE:HG23	2:H:943:LEU:HD11	1.78	0.65
1:A:940:THR:O	1:A:944:ARG:HG3	1.97	0.65
1:E:950:LEU:HD12	1:E:959:ILE:HD13	1.79	0.65
1:G:395:LEU:CD1	1:G:400:ASP:HB2	2.27	0.65
1:G:650:ALA:HB2	1:G:666:TYR:HB2	1.79	0.65
1:G:839:GLN:HB2	1:G:841:TYR:HD1	1.60	0.65
1:E:351:ALA:HA	1:E:380:ILE:HD12	1.78	0.65
1:G:973:LEU:O	1:G:980:LEU:HD22	1.97	0.65
1:A:842:LYS:NZ	1:A:919:GLY:HA2	2.12	0.64
1:G:408:TYR:O	1:G:412:ILE:HG12	1.97	0.64
1:E:990:GLN:O	1:E:994:SER:HB3	1.97	0.64
1:C:406:GLN:O	1:C:410:ARG:HD3	1.97	0.64



	lo uo pago	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:953:LEU:O	1:E:990:GLN:HG3	1.97	0.64
1:C:866:LEU:HD13	1:C:893:SER:O	1.98	0.64
1:C:660:GLY:HA2	1:C:683:SER:HB3	1.80	0.64
1:G:555:PHE:O	1:G:592:ARG:HD2	1.98	0.64
1:G:576:PHE:CE2	1:G:1007:GLU:HB3	2.33	0.64
1:G:900:GLU:O	1:G:904:ARG:HG2	1.98	0.64
1:A:405:LEU:HD13	1:A:428:ILE:CD1	2.28	0.64
1:A:710:VAL:HG11	1:A:721:ASP:HA	1.80	0.64
1:A:362:GLN:NE2	1:A:370:ALA:HB1	2.11	0.63
1:A:1001:GLN:O	1:A:1005:GLU:HG3	1.97	0.63
1:A:535:HIS:HE1	1:A:644:ARG:HG3	1.63	0.63
1:G:1000:LYS:O	1:G:1004:MET:HG3	1.97	0.63
1:A:405:LEU:HD13	1:A:428:ILE:HD11	1.79	0.63
1:E:344:LEU:HD22	1:E:353:ALA:HB1	1.79	0.63
1:E:927:LEU:HG	1:E:933:MET:HE2	1.79	0.63
1:G:395:LEU:HD23	1:G:404:ALA:N	2.13	0.63
1:G:449:LYS:HE3	1:G:452:PHE:HD1	1.62	0.63
1:A:502:LEU:HD11	1:A:841:TYR:CD1	2.33	0.63
1:E:777:ILE:CG2	2:F:943:LEU:HB3	2.28	0.63
1:G:490:ASN:HA	1:G:516:ARG:HH22	1.63	0.63
1:A:327:LYS:HD2	1:A:332:ASN:ND2	2.13	0.63
1:A:805:ASN:O	1:A:809:THR:HG23	1.98	0.63
1:C:324:ALA:HB2	1:C:339:LEU:HB3	1.81	0.63
1:C:828:PRO:CG	1:C:831:ALA:HB3	2.27	0.63
1:G:324:ALA:HB2	1:G:339:LEU:CB	2.28	0.63
2:H:938:SER:HB2	2:H:939:PRO:CD	2.29	0.63
1:A:326:ILE:O	1:A:330:GLN:HG2	1.98	0.63
1:E:357:LEU:O	1:E:360:VAL:HG22	1.99	0.63
1:E:798:LEU:CD1	1:E:824:GLN:HB3	2.22	0.63
1:G:924:MET:HE3	1:G:997:PHE:CE1	2.33	0.63
1:A:564:MET:HA	1:A:567:ILE:CD1	2.29	0.63
1:A:941:LEU:O	1:A:945:VAL:HG23	1.99	0.63
1:A:564:MET:O	1:A:564:MET:HE2	1.99	0.63
1:E:506:SER:HG	1:E:509:PHE:HD1	1.47	0.62
1:G:592:ARG:O	1:G:596:MET:HG3	1.99	0.62
1:C:374:TYR:HB3	1:C:391:MET:HE3	1.80	0.62
1:C:378:ILE:CD1	1:C:388:TYR:HD2	2.12	0.62
1:G:797:GLY:HA2	1:G:818:ILE:HG23	1.81	0.62
1:A:444:THR:O	1:A:448:LEU:HG	1.99	0.62
1:A:723:ARG:NH2	1:A:829:GLU:HB3	2.14	0.62
1:E:497:PRO:HD3	1:E:517:HIS:CE1	2.35	0.62



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:853:ASN:O	1:G:857:ARG:HG3	1.99	0.62
1:G:854:ILE:HD13	1:G:970:ALA:CB	2.29	0.62
1:A:320:LEU:HD22	1:A:342:LYS:HB3	1.81	0.62
1:A:668:ILE:HA	1:A:687:ALA:HB3	1.81	0.62
1:C:479:LEU:O	1:C:483:VAL:HG23	1.99	0.62
1:G:651:MET:SD	1:G:659:SER:HB3	2.40	0.62
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.35	0.62
1:A:479:LEU:O	1:A:483:VAL:HG23	2.00	0.62
1:A:898:LYS:O	1:A:902:VAL:HG23	2.00	0.62
1:E:426:ALA:HB3	1:E:442:TYR:CD1	2.35	0.62
1:C:371:LEU:HD11	1:C:395:LEU:CD2	2.30	0.62
1:A:384:PHE:HD2	1:A:387:ALA:HB2	1.64	0.62
1:C:720:TYR:HD2	1:C:723:ARG:CD	2.12	0.62
1:C:376:GLU:O	1:C:379:ARG:HG3	2.00	0.61
1:E:823:SER:HA	2:F:941:TYR:CE2	2.35	0.61
1:G:610:CYS:HB3	1:G:613:LYS:HD2	1.81	0.61
1:A:486:GLN:OE1	1:A:493:PRO:HA	2.00	0.61
1:C:405:LEU:HD13	1:C:428:ILE:HD13	1.80	0.61
1:C:831:ALA:HB1	1:C:860:ASN:O	2.00	0.61
1:G:942:ALA:O	1:G:945:VAL:HG22	2.00	0.61
1:C:553:SER:HB3	1:C:583:LEU:HB2	1.81	0.61
1:C:669:THR:O	1:C:688:TYR:HA	2.01	0.61
1:C:670:ASP:OD2	1:C:692:THR:HA	1.98	0.61
1:G:476:MET:CE	1:G:504:PRO:HD2	2.29	0.61
1:A:984:ARG:HG2	1:A:984:ARG:HH11	1.65	0.61
1:C:350:PHE:HD1	1:C:353:ALA:H	1.47	0.61
1:A:323:LEU:HD22	1:A:339:LEU:HG	1.81	0.61
1:E:512:ALA:O	1:E:516:ARG:HG2	2.00	0.61
1:E:596:MET:HG2	1:E:602:PHE:CD2	2.35	0.61
1:A:838:ASN:HD21	1:A:919:GLY:HA3	1.65	0.61
1:C:557:ASN:HB2	1:C:589:THR:HG21	1.80	0.61
1:G:374:TYR:HB3	1:G:391:MET:HG2	1.83	0.61
1:A:853:ASN:O	1:A:857:ARG:HG3	2.01	0.61
1:E:831:ALA:HB1	1:E:860:ASN:O	2.01	0.61
1:A:324:ALA:HB2	1:A:339:LEU:HB3	1.83	0.60
1:A:388:TYR:HB3	1:A:411:ALA:HB2	1.81	0.60
1:A:453:PRO:HB3	1:A:482:ILE:HG21	1.82	0.60
1:E:726:LEU:HG	1:E:819:VAL:HG22	1.83	0.60
2:H:942:LEU:H	2:H:942:LEU:CD2	2.14	0.60
1:A:660:GLY:HA2	1:A:683:SER:HB3	1.82	0.60
1:C:322:ASN:O	1:C:326:ILE:HG13	2.01	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:723:ARG:O	1:G:724:ILE:HD13	2.01	0.60
1:G:886:PRO:HG2	1:G:889:ARG:HG2	1.84	0.60
1:C:685:LYS:HD3	1:C:1025:HIS:CE1	2.36	0.60
1:A:395:LEU:HD12	1:A:398:MET:HE2	1.82	0.60
1:A:457:CYS:SG	1:A:494:SER:HB2	2.42	0.60
1:G:1007:GLU:O	1:G:1011:LEU:HG	2.01	0.60
1:A:920:HIS:HE1	1:A:942:ALA:HA	1.66	0.60
1:C:332:ASN:HD22	1:C:335:GLU:HB3	1.65	0.60
1:A:920:HIS:CD2	3:A:1201:UD1:HN2'	2.20	0.60
1:C:358:ALA:HB2	1:C:373:HIS:HB2	1.82	0.60
1:E:828:PRO:CG	1:E:831:ALA:HB3	2.31	0.60
1:G:670:ASP:O	1:G:673:THR:HB	2.02	0.60
1:E:850:MET:HE3	1:E:967:GLU:HG3	1.83	0.60
1:G:374:TYR:HB3	1:G:391:MET:CG	2.32	0.60
1:G:920:HIS:HE1	3:G:1201:UD1:H8'2	1.66	0.60
1:A:357:LEU:HD13	1:A:373:HIS:HE1	1.66	0.59
1:C:324:ALA:HA	1:C:339:LEU:HD12	1.83	0.59
1:E:338:ARG:O	1:E:342:LYS:HG2	2.01	0.59
1:E:340:TYR:O	1:E:344:LEU:HD23	2.02	0.59
1:E:712:ASP:CA	1:E:719:ILE:HD11	2.20	0.59
1:G:820:THR:HG22	1:G:907:LEU:HD11	1.83	0.59
1:G:770:ASN:O	1:G:774:GLU:HG3	2.01	0.59
1:E:911:CYS:O	1:E:933:MET:HA	2.02	0.59
1:E:376:GLU:O	1:E:380:ILE:HG13	2.03	0.59
1:E:920:HIS:CD2	1:E:945:VAL:HG21	2.38	0.59
1:G:333:ILE:HG22	1:G:364:GLN:HE22	1.67	0.59
1:G:476:MET:HE2	1:G:504:PRO:CD	2.31	0.59
1:G:565:GLN:HB2	1:G:594:LYS:HD2	1.85	0.59
1:A:335:GLU:HA	1:A:338:ARG:HD3	1.85	0.59
1:A:418:PHE:HD1	1:A:421:ALA:H	1.51	0.59
1:G:395:LEU:HD11	1:G:400:ASP:HB2	1.84	0.59
1:G:822:ARG:HB3	1:G:827:LEU:HB2	1.84	0.59
1:E:350:PHE:CE1	1:E:352:ALA:HB3	2.37	0.59
1:E:806:LYS:HD3	1:E:811:GLU:HB2	1.84	0.59
1:E:953:LEU:HD13	1:E:996:LEU:CD2	2.33	0.59
1:A:476:MET:O	1:A:480:VAL:HG23	2.03	0.59
1:A:1025:HIS:HB3	1:A:1027:ILE:HD11	1.84	0.59
1:C:323:LEU:O	1:C:327:LYS:HG2	2.03	0.59
1:C:379:ARG:CZ	1:C:380:ILE:HG12	2.33	0.59
1:C:720:TYR:HD2	1:C:723:ARG:HD3	1.67	0.59
1:C:787:ILE:HG13	1:C:794:ILE:HB	1.85	0.59



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:408:TYR:O	1:E:412:ILE:HG13	2.03	0.59
1:E:449:LYS:HE3	1:E:452:PHE:CD1	2.38	0.59
1:A:502:LEU:HA	1:A:916:LEU:HD11	1.85	0.58
1:A:1022:LYS:HB3	1:A:1023:PRO:HD2	1.84	0.58
1:C:855:LEU:O	1:C:889:ARG:NH2	2.35	0.58
1:G:320:LEU:HD12	1:G:343:ALA:CA	2.33	0.58
1:G:361:LEU:HB2	1:G:370:ALA:HB2	1.83	0.58
1:G:842:LYS:HG2	1:G:917:CYS:HB2	1.83	0.58
1:E:714:LYS:HZ1	2:F:946:PRO:HB2	1.69	0.58
1:G:834:TYR:O	1:G:863:LEU:HD12	2.03	0.58
1:A:534:GLU:HA	1:A:534:GLU:OE1	2.03	0.58
1:A:358:ALA:HA	1:A:361:LEU:HB2	1.85	0.58
1:E:868:PHE:CD1	1:E:895:VAL:HG21	2.38	0.58
1:E:886:PRO:HG2	1:E:889:ARG:HG2	1.85	0.58
1:G:854:ILE:HD13	1:G:970:ALA:HB3	1.86	0.58
1:C:693:PHE:CG	1:C:693:PHE:O	2.57	0.58
1:E:688:TYR:CD2	1:E:1027:ILE:HD13	2.39	0.58
1:E:779:MET:SD	1:E:787:ILE:HG23	2.44	0.58
1:C:426:ALA:HB2	1:C:441:SER:CB	2.33	0.58
1:C:695:ILE:HB	1:C:1002:TYR:CD2	2.39	0.58
1:E:950:LEU:HD12	1:E:959:ILE:CD1	2.34	0.58
1:C:576:PHE:CE2	1:C:1007:GLU:HB3	2.39	0.58
1:A:357:LEU:O	1:A:357:LEU:HD23	2.03	0.58
1:C:364:GLN:O	1:C:524:LYS:HA	2.04	0.58
1:E:361:LEU:HB2	1:E:370:ALA:HB2	1.85	0.58
1:E:457:CYS:SG	1:E:494:SER:HB2	2.44	0.58
1:C:361:LEU:HB3	1:C:370:ALA:HB2	1.86	0.58
1:E:690:PRO:HG2	1:E:1005:GLU:OE1	2.04	0.58
1:E:822:ARG:HD3	1:E:827:LEU:CB	2.33	0.58
1:E:868:PHE:HD1	1:E:895:VAL:HG21	1.69	0.57
1:G:369:GLU:CD	1:G:369:GLU:H	2.06	0.57
1:A:895:VAL:HG13	3:A:1201:UD1:C4	2.33	0.57
1:E:644:ARG:HA	1:E:649:GLN:OE1	2.04	0.57
1:G:320:LEU:HB2	1:G:343:ALA:HB2	1.86	0.57
1:A:675:PRO:HD2	1:A:678:VAL:HG11	1.87	0.57
1:A:821:THR:CG2	1:A:824:GLN:HG3	2.34	0.57
1:C:913:ASP:O	1:C:915:PRO:HD3	2.05	0.57
1:E:652:TRP:NE1	1:E:653:LEU:HD13	2.19	0.57
1:G:559:PRO:CB	3:G:1201:UD1:H6'2	2.30	0.57
1:C:342:LYS:HA	1:C:345:GLU:OE1	2.04	0.57
1:C:669:THR:HA	1:C:693:PHE:CG	2.38	0.57



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:449:LYS:HE3	1:A:452:PHE:CD1	2.39	0.57
1:A:632:TYR:HE1	1:A:659:SER:HA	1.69	0.57
1:C:435:ILE:HD12	1:C:435:ILE:H	1.69	0.57
1:C:538:ASP:OD2	1:C:540:LYS:HD2	2.04	0.57
1:G:358:ALA:HB2	1:G:373:HIS:HB2	1.86	0.57
1:C:357:LEU:HD23	1:C:373:HIS:CE1	2.40	0.57
1:C:983:VAL:O	1:C:987:VAL:HG23	2.05	0.57
1:E:415:ASN:ND2	1:E:418:PHE:HB2	2.20	0.57
1:G:719:ILE:HG13	1:G:720:TYR:H	1.69	0.57
1:G:731:LEU:O	1:G:735:LEU:HG	2.05	0.57
1:A:358:ALA:HB3	1:A:374:TYR:CE1	2.40	0.57
1:G:403:GLY:HA2	1:G:406:GLN:HB3	1.85	0.57
1:G:415:ASN:ND2	1:G:418:PHE:HB2	2.20	0.57
1:A:562:HIS:ND1	1:A:898:LYS:HE2	2.20	0.56
1:C:502:LEU:HA	1:C:916:LEU:HD11	1.87	0.56
1:G:697:ASP:OD1	1:G:700:ASN:HB3	2.04	0.56
1:A:361:LEU:HD13	1:A:369:GLU:HG2	1.86	0.56
1:C:358:ALA:HB1	1:C:374:TYR:CE2	2.40	0.56
1:C:480:VAL:HG22	1:C:505:LEU:HD23	1.87	0.56
1:E:479:LEU:O	1:E:483:VAL:HG23	2.05	0.56
1:E:854:ILE:HD13	1:E:970:ALA:CB	2.35	0.56
1:A:1008:ARG:O	1:A:1012:GLN:HG3	2.05	0.56
1:E:317:ALA:HB2	1:E:346:VAL:HB	1.87	0.56
1:E:927:LEU:HD22	1:E:953:LEU:HD22	1.85	0.56
1:G:913:ASP:O	1:G:915:PRO:HD3	2.04	0.56
1:A:341:ARG:O	1:A:345:GLU:HG2	2.05	0.56
1:G:624:HIS:O	1:G:647:PRO:HG2	2.04	0.56
1:G:879:TYR:O	1:G:883:MET:HG3	2.06	0.56
1:C:357:LEU:O	1:C:361:LEU:HD13	2.06	0.56
1:C:879:TYR:O	1:C:883:MET:HG3	2.04	0.56
1:G:367:LEU:HD21	1:G:397:GLU:HG2	1.86	0.56
1:A:838:ASN:HB3	1:A:842:LYS:HD2	1.86	0.56
1:C:522:LEU:HD21	1:C:663:PHE:CE1	2.41	0.56
1:E:668:ILE:HD13	1:E:687:ALA:HB3	1.86	0.56
1:G:490:ASN:CA	1:G:516:ARG:HH22	2.17	0.56
1:C:918:ASN:HB2	1:C:942:ALA:O	2.05	0.56
1:G:452:PHE:HD2	1:G:455:ALA:HB3	1.71	0.56
1:E:827:LEU:HD11	1:E:864:TRP:CE3	2.41	0.56
1:G:457:CYS:SG	1:G:494:SER:HB2	2.46	0.56
1:A:719:ILE:HG23	1:A:744:VAL:HG11	1.88	0.56
1:C:492:LEU:HD12	1:C:493:PRO:HD2	1.87	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:538:ASP:OD2	1:E:540:LYS:HD2	2.06	0.56
1:G:342:LYS:O	1:G:346:VAL:HG23	2.06	0.56
1:G:366:LYS:HE3	1:G:369:GLU:OE2	2.06	0.56
1:G:777:ILE:CG2	2:H:943:LEU:HD11	2.36	0.56
1:C:327:LYS:HB2	1:C:336:ALA:HB2	1.88	0.55
1:C:631:GLY:HA3	1:C:655:TYR:HB2	1.87	0.55
1:E:426:ALA:HB3	1:E:442:TYR:CE1	2.41	0.55
1:A:335:GLU:HB3	1:A:338:ARG:NH1	2.16	0.55
1:A:975:THR:HG21	1:G:488:GLU:OE2	2.06	0.55
1:E:340:TYR:HB2	1:E:357:LEU:HD13	1.88	0.55
1:E:854:ILE:HD13	1:E:970:ALA:HB3	1.88	0.55
1:A:521:CYS:O	1:A:524:LYS:HG2	2.07	0.55
1:E:820:THR:HG22	1:E:907:LEU:HD11	1.87	0.55
1:E:826:GLY:CA	2:F:940:LYS:HE3	2.29	0.55
1:E:839:GLN:HB3	1:E:841:TYR:HD2	1.71	0.55
1:G:323:LEU:O	1:G:326:ILE:HG12	2.07	0.55
1:G:361:LEU:CB	1:G:370:ALA:HB2	2.36	0.55
1:A:374:TYR:CE2	1:A:390:ASN:HB3	2.42	0.55
1:A:560:THR:O	1:A:564:MET:HG3	2.06	0.55
1:A:984:ARG:HG2	1:A:984:ARG:NH1	2.21	0.55
1:A:1026:MET:C	1:A:1027:ILE:HD12	2.27	0.55
1:E:901:HIS:HA	1:E:904:ARG:HE	1.70	0.55
1:A:419:ALA:HA	1:A:448:LEU:HD12	1.86	0.55
1:C:868:PHE:CD1	1:C:895:VAL:HG21	2.42	0.55
1:E:432:SER:OG	1:G:383:THR:HG21	2.06	0.55
1:E:913:ASP:OD2	1:E:933:MET:HG2	2.06	0.55
1:G:947:ALA:O	1:G:951:THR:HG23	2.07	0.55
1:A:685:LYS:HE3	1:A:1024:ASP:HA	1.87	0.55
1:C:320:LEU:HD12	1:C:343:ALA:HA	1.88	0.55
1:G:554:ASP:HB3	1:G:558:HIS:CG	2.42	0.55
1:A:521:CYS:HA	1:A:524:LYS:CD	2.37	0.55
1:A:807:ALA:HA	1:A:812:GLU:O	2.08	0.55
1:E:826:GLY:HA2	2:F:941:TYR:HD2	1.72	0.55
1:G:426:ALA:HB2	1:G:441:SER:CB	2.35	0.55
1:G:552:SER:HA	1:G:630:ASN:OD1	2.07	0.55
1:A:689:MET:CE	1:A:690:PRO:HD2	2.37	0.54
1:C:823:SER:CB	2:D:943:LEU:HD21	2.37	0.54
1:G:614:ALA:O	1:G:618:ILE:HD12	2.06	0.54
1:G:896:ALA:HB2	1:G:904:ARG:NH2	2.22	0.54
1:A:658:THR:HG21	1:A:681:GLN:O	2.06	0.54
1:C:1000:LYS:O	1:C:1004:MET:HG3	2.07	0.54



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:783:GLY:HA3	2:H:938:SER:HB3	1.89	0.54
1:G:1011:LEU:O	1:G:1015:GLU:HG2	2.06	0.54
1:A:553:SER:HB3	1:A:583:LEU:HB2	1.87	0.54
1:C:419:ALA:HB2	1:C:448:LEU:HB2	1.88	0.54
1:E:738:LEU:HB2	1:E:741:VAL:CG2	2.37	0.54
1:E:839:GLN:HB3	1:E:841:TYR:CD2	2.42	0.54
1:C:388:TYR:OH	1:C:414:ILE:HD12	2.08	0.54
1:C:555:PHE:O	1:C:592:ARG:HD3	2.07	0.54
1:C:594:LYS:O	1:C:598:GLU:HG3	2.07	0.54
1:E:492:LEU:CD1	1:E:520:LEU:HD11	2.38	0.54
1:E:872:GLY:O	1:E:876:ILE:HG12	2.07	0.54
1:G:344:LEU:O	1:G:344:LEU:HD23	2.08	0.54
1:A:354:HIS:CE1	1:A:376:GLU:HG2	2.43	0.54
1:A:517:HIS:HA	1:A:520:LEU:HG	1.90	0.54
1:C:769:MET:CE	2:D:945:LEU:HB2	2.37	0.54
1:E:734:PHE:CE1	1:E:738:LEU:HD11	2.43	0.54
1:E:1011:LEU:O	1:E:1015:GLU:HG2	2.06	0.54
1:G:545:ARG:HD2	1:G:573:PRO:O	2.07	0.54
1:E:425:LEU:O	1:E:428:ILE:HG13	2.07	0.54
1:G:389:SER:HB2	1:G:424:ASN:OD1	2.08	0.54
1:G:449:LYS:HE3	1:G:452:PHE:CD1	2.40	0.54
1:G:496:HIS:CG	1:G:497:PRO:HD2	2.41	0.54
1:G:941:LEU:O	1:G:945:VAL:HG13	2.08	0.54
1:A:434:ASN:OD1	1:A:437:GLU:HB2	2.07	0.54
1:A:730:ASP:OD2	1:C:1000:LYS:HE2	2.07	0.54
1:A:804:ASN:ND2	1:A:807:ALA:HB2	2.23	0.54
2:B:938:SER:CB	2:B:939:PRO:HD2	2.38	0.54
1:C:807:ALA:HA	1:C:812:GLU:O	2.08	0.54
1:E:432:SER:CB	1:G:383:THR:HG21	2.38	0.54
1:G:332:ASN:ND2	1:G:335:GLU:HB2	2.23	0.54
1:G:855:LEU:HD12	1:G:885:LEU:HD11	1.89	0.54
1:C:590:ASN:ND2	1:C:811:GLU:HB3	2.22	0.54
1:C:823:SER:HA	2:D:941:TYR:CE2	2.43	0.54
1:C:950:LEU:HD13	1:C:958:LEU:HB2	1.89	0.54
1:E:672:GLU:HG2	1:E:951:THR:HG21	1.90	0.54
1:G:583:LEU:HD22	1:G:637:ARG:HD3	1.90	0.54
1:A:1011:LEU:O	1:A:1015:GLU:HG2	2.07	0.54
1:C:342:LYS:O	1:C:346:VAL:HG23	2.08	0.54
1:E:469:TRP:CH2	1:E:843:ILE:HG22	2.43	0.54
1:A:374:TYR:HD2	1:A:391:MET:HA	1.74	0.53
1:A:720:TYR:CD2	1:A:723:ARG:HD3	2.43	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:632:TYR:HB2	1:C:655:TYR:CE2	2.43	0.53
1:E:466:VAL:HG12	1:E:871:VAL:CG2	2.38	0.53
1:E:547:ARG:HH11	1:E:622:GLY:HA3	1.73	0.53
1:E:804:ASN:ND2	1:E:807:ALA:HB2	2.23	0.53
1:G:963:ARG:HD3	1:G:963:ARG:N	2.23	0.53
1:C:652:TRP:CD1	1:C:653:LEU:HD13	2.43	0.53
1:E:378:ILE:HD11	1:E:387:ALA:HB3	1.89	0.53
1:E:712:ASP:O	1:E:769:MET:HG2	2.08	0.53
1:E:768:PRO:HG2	1:E:770:ASN:ND2	2.22	0.53
1:G:452:PHE:HD2	1:G:455:ALA:CB	2.21	0.53
1:G:692:THR:HG21	1:G:996:LEU:CD1	2.38	0.53
1:A:419:ALA:HB2	1:A:448:LEU:HB2	1.90	0.53
1:E:658:THR:HB	1:E:682:TYR:HA	1.90	0.53
1:E:685:LYS:HE3	1:E:1024:ASP:HA	1.90	0.53
1:G:720:TYR:CD2	1:G:723:ARG:HD3	2.44	0.53
1:A:652:TRP:CD1	1:A:668:ILE:HD12	2.42	0.53
1:G:847:THR:HG23	1:G:915:PRO:HD2	1.91	0.53
1:A:780:ILE:HG21	1:A:821:THR:HG21	1.90	0.53
1:E:367:LEU:HD13	1:E:398:MET:SD	2.48	0.53
1:G:685:LYS:HD3	1:G:1025:HIS:CE1	2.43	0.53
1:G:965:GLU:O	1:G:969:ILE:HG12	2.09	0.53
1:E:650:ALA:HB2	1:E:666:TYR:HB2	1.91	0.53
1:A:469:TRP:CD2	1:A:845:PRO:HG3	2.44	0.53
1:C:358:ALA:HB1	1:C:374:TYR:CD2	2.44	0.53
1:C:427:SER:O	1:C:430:LYS:HB3	2.08	0.53
1:C:828:PRO:HG2	1:C:831:ALA:HB3	1.91	0.53
1:C:921:THR:N	3:C:1201:UD1:O2B	2.42	0.53
1:G:533:TYR:HB3	1:G:619:HIS:NE2	2.24	0.53
1:G:846:SER:O	1:G:850:MET:HG3	2.09	0.53
1:A:608:ILE:CG2	1:A:613:LYS:HG2	2.39	0.53
1:C:351:ALA:H	1:C:354:HIS:HD2	1.57	0.53
1:E:418:PHE:CZ	1:E:420:ASP:HB2	2.44	0.53
1:A:344:LEU:HD12	1:A:353:ALA:HB1	1.90	0.53
1:A:352:ALA:O	1:A:356:ASN:ND2	2.42	0.53
1:C:690:PRO:HG2	1:C:1005:GLU:CD	2.30	0.53
1:E:510:ARG:HA	1:E:513:ILE:HD12	1.91	0.53
1:A:779:MET:CE	1:A:794:ILE:HG22	2.39	0.52
1:C:670:ASP:CG	1:C:692:THR:HA	2.29	0.52
1:C:823:SER:HB3	2:D:943:LEU:HD21	1.90	0.52
1:C:886:PRO:HG2	1:C:889:ARG:HG2	1.91	0.52
1:A:512:ALA:O	1:A:516:ARG:HG2	2.08	0.52



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:344:LEU:HD11	1:C:354:HIS:NE2	2.24	0.52
1:E:551:VAL:HG22	1:E:581:TYR:HB2	1.91	0.52
1:C:660:GLY:HA2	1:C:683:SER:CB	2.39	0.52
1:G:324:ALA:N	1:G:339:LEU:HD22	2.24	0.52
2:H:938:SER:HB2	2:H:939:PRO:HD2	1.91	0.52
1:E:476:MET:O	1:E:480:VAL:HG23	2.10	0.52
1:A:521:CYS:CB	1:A:639:GLU:HG3	2.39	0.52
1:E:564:MET:CA	1:E:567:ILE:HD13	2.40	0.52
1:E:580:CYS:HB2	1:E:602:PHE:HD1	1.74	0.52
1:E:806:LYS:HD2	1:E:811:GLU:CB	2.39	0.52
1:A:333:ILE:HD11	1:A:360:VAL:HB	1.92	0.52
1:E:995:PRO:HB3	1:E:1001:GLN:OE1	2.10	0.52
1:G:833:VAL:HG23	1:G:909:ASP:H	1.75	0.52
1:G:963:ARG:H	1:G:963:ARG:CD	2.21	0.52
1:C:742:LYS:O	1:C:743:ILE:HD13	2.10	0.52
1:E:828:PRO:HG2	1:E:831:ALA:HB3	1.91	0.52
1:G:480:VAL:HG22	1:G:505:LEU:HD23	1.91	0.52
1:A:461:HIS:O	1:A:465:ILE:HG13	2.09	0.52
1:C:371:LEU:HD23	1:C:371:LEU:O	2.10	0.52
1:C:446:LEU:HD23	1:C:452:PHE:HB3	1.92	0.52
1:A:344:LEU:CD1	1:A:353:ALA:HB1	2.39	0.52
1:C:979:TYR:O	1:C:983:VAL:HG23	2.09	0.52
1:G:798:LEU:O	1:G:798:LEU:HD23	2.10	0.52
1:G:898:LYS:NZ	3:G:1201:UD1:H1B	2.25	0.52
1:A:626:LEU:HG	1:A:641:PHE:CZ	2.45	0.52
1:A:842:LYS:HZ3	1:A:919:GLY:HA2	1.75	0.52
1:A:722:ASN:OD1	1:A:822:ARG:NH2	2.44	0.51
1:C:374:TYR:CG	1:C:391:MET:HB2	2.45	0.51
1:A:800:THR:HA	1:A:803:ILE:CG2	2.39	0.51
1:A:836:ASN:HD21	1:A:838:ASN:HD22	1.57	0.51
1:E:511:LYS:HD3	1:E:680:GLU:O	2.09	0.51
1:G:317:ALA:HA	1:G:320:LEU:HG	1.92	0.51
1:G:828:PRO:HG2	1:G:831:ALA:HB3	1.92	0.51
1:G:695:ILE:HG13	1:G:696:GLY:H	1.74	0.51
1:E:818:ILE:HG21	1:E:903:ARG:HD2	1.92	0.51
1:E:918:ASN:O	1:E:920:HIS:ND1	2.44	0.51
1:A:333:ILE:O	1:A:337:VAL:HG12	2.11	0.51
1:A:650:ALA:HB2	1:A:666:TYR:HB2	1.92	0.51
1:A:834:TYR:CD1	1:A:912:LEU:HD21	2.45	0.51
1:C:779:MET:HE1	1:C:794:ILE:HG22	1.91	0.51
1:E:922:THR:O	1:E:926:VAL:HG12	2.11	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:358:ALA:HB3	1:A:374:TYR:CD1	2.46	0.51
1:A:918:ASN:HB2	1:A:942:ALA:O	2.10	0.51
1:C:694:PHE:CZ	1:C:920:HIS:HB3	2.46	0.51
1:E:711:ILE:HG12	1:E:767:ILE:HB	1.93	0.51
1:G:834:TYR:O	1:G:863:LEU:HA	2.11	0.51
1:A:453:PRO:HB3	1:A:482:ILE:CG2	2.40	0.51
1:C:324:ALA:HB2	1:C:339:LEU:HB2	1.92	0.51
1:C:405:LEU:HD13	1:C:428:ILE:HD11	1.91	0.51
1:E:713:PHE:O	1:E:714:LYS:HB3	2.10	0.51
1:E:793:SER:O	1:E:794:ILE:HD13	2.11	0.51
1:A:535:HIS:CE1	1:A:644:ARG:HG3	2.45	0.51
1:E:514:ALA:HB1	1:E:659:SER:O	2.11	0.51
1:E:564:MET:HA	1:E:567:ILE:HD13	1.93	0.51
1:E:669:THR:O	1:E:688:TYR:HA	2.11	0.51
1:A:921:THR:N	3:A:1201:UD1:O2B	2.43	0.51
1:E:567:ILE:H	1:E:567:ILE:HD12	1.76	0.51
1:E:918:ASN:HB3	1:E:946:ALA:H	1.75	0.51
1:G:408:TYR:CZ	1:G:424:ASN:HB3	2.45	0.51
1:A:821:THR:HG22	1:A:824:GLN:HG3	1.94	0.50
1:E:835:CYS:O	1:E:911:CYS:HA	2.11	0.50
1:A:800:THR:O	1:A:803:ILE:HG22	2.10	0.50
1:A:990:GLN:HA	1:A:993:SER:OG	2.11	0.50
1:G:350:PHE:CD2	1:G:353:ALA:HB2	2.47	0.50
1:G:818:ILE:HG21	1:G:903:ARG:CZ	2.42	0.50
1:C:823:SER:HA	2:D:941:TYR:CZ	2.46	0.50
1:C:953:LEU:HD12	1:C:994:SER:OG	2.11	0.50
1:G:535:HIS:ND1	1:G:647:PRO:HA	2.27	0.50
1:C:502:LEU:HD21	1:C:841:TYR:HE2	1.76	0.50
1:E:779:MET:SD	1:E:787:ILE:HG12	2.51	0.50
1:E:953:LEU:HD13	1:E:996:LEU:HD23	1.92	0.50
1:E:988:TRP:HA	1:E:991:ARG:HD3	1.93	0.50
1:C:675:PRO:O	1:C:678:VAL:HG22	2.11	0.50
1:E:507:HIS:NE2	1:E:939:GLU:HB3	2.26	0.50
1:E:555:PHE:O	1:E:592:ARG:HD2	2.12	0.50
1:A:567:ILE:HD12	1:A:567:ILE:H	1.76	0.50
1:E:559:PRO:HB2	3:E:1201:UD1:H6'2	1.94	0.50
1:C:871:VAL:O	1:C:874:PRO:HD2	2.12	0.50
1:A:395:LEU:HB3	1:A:404:ALA:HB2	1.93	0.50
1:A:564:MET:CA	1:A:567:ILE:HD13	2.41	0.50
1:C:428:ILE:HG13	1:C:429:HIS:N	2.27	0.50
1:E:466:VAL:HG12	1:E:871:VAL:HG23	1.94	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:533:TYR:HB3	1:G:619:HIS:CD2	2.47	0.50
1:A:388:TYR:CB	1:A:411:ALA:HB2	2.41	0.50
1:C:476:MET:O	1:C:480:VAL:HG23	2.11	0.50
1:E:374:TYR:CB	1:E:391:MET:HE2	2.35	0.50
1:E:687:ALA:HB1	1:E:1009:LEU:HD21	1.94	0.50
1:E:781:ASN:HA	2:F:939:PRO:HG3	1.93	0.50
1:G:412:ILE:HG23	1:G:422:HIS:CE1	2.47	0.50
1:G:836:ASN:HD21	1:G:914:THR:HG22	1.76	0.50
1:C:514:ALA:HB1	1:C:659:SER:O	2.12	0.49
1:E:806:LYS:HD2	1:E:811:GLU:HB2	1.94	0.49
1:E:827:LEU:HD13	1:E:833:VAL:HG11	1.94	0.49
1:C:418:PHE:HD2	1:C:421:ALA:H	1.60	0.49
1:C:457:CYS:SG	1:C:494:SER:HB2	2.52	0.49
1:E:726:LEU:CD2	1:E:819:VAL:HG22	2.42	0.49
1:E:918:ASN:HB2	1:E:942:ALA:O	2.12	0.49
1:C:385:ALA:O	1:C:389:SER:HB3	2.11	0.49
1:E:442:TYR:CE2	1:E:458:ASN:HB3	2.48	0.49
1:E:937:PRO:HA	1:E:943:SER:O	2.12	0.49
1:G:366:LYS:HG3	1:G:369:GLU:OE2	2.11	0.49
1:G:839:GLN:HG2	1:G:868:PHE:HE2	1.78	0.49
1:A:320:LEU:HB2	1:A:343:ALA:HB2	1.94	0.49
1:A:374:TYR:CZ	1:A:390:ASN:HB3	2.48	0.49
1:C:834:TYR:CD2	1:C:912:LEU:HD21	2.47	0.49
3:C:1201:UD1:N2'	3:C:1201:UD1:O1B	2.44	0.49
1:G:327:LYS:HE2	1:G:335:GLU:CG	2.43	0.49
1:G:333:ILE:CG2	1:G:364:GLN:HE22	2.25	0.49
1:G:515:GLU:HA	1:G:660:GLY:O	2.13	0.49
1:C:746:MET:CE	1:C:762:LEU:HA	2.42	0.49
1:C:769:MET:HE2	2:D:946:PRO:HD2	1.93	0.49
1:G:836:ASN:HD21	1:G:914:THR:CG2	2.25	0.49
1:G:901:HIS:HB2	3:G:1201:UD1:N3	2.27	0.49
1:A:359:SER:O	1:A:362:GLN:HG2	2.13	0.49
1:C:779:MET:CE	1:C:794:ILE:HG22	2.43	0.49
1:E:320:LEU:HB2	1:E:343:ALA:HB2	1.93	0.49
1:E:669:THR:CG2	1:E:686:LEU:HD22	2.40	0.49
1:E:950:LEU:HB2	1:E:959:ILE:HD11	1.93	0.49
1:G:525:ILE:HD12	1:G:643:LEU:HD23	1.93	0.49
1:A:321:ASN:HD21	1:A:356:ASN:HD21	1.61	0.49
1:C:425:LEU:O	1:C:428:ILE:HG12	2.13	0.49
1:E:564:MET:CB	1:E:567:ILE:HD13	2.43	0.49
1:C:937:PRO:HA	1:C:943:SER:O	2.13	0.49



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:452:PHE:HD2	1:E:455:ALA:CB	2.25	0.49
1:E:652:TRP:CE2	1:E:653:LEU:HD13	2.48	0.49
1:G:374:TYR:CB	1:G:391:MET:HG2	2.43	0.49
1:A:359:SER:CA	1:A:362:GLN:HG2	2.41	0.49
1:A:522:LEU:O	1:A:525:ILE:HG12	2.12	0.49
1:A:854:ILE:CD1	1:A:970:ALA:HB3	2.42	0.49
1:G:967:GLU:O	1:G:971:VAL:HG23	2.13	0.49
1:A:557:ASN:HB2	1:A:589:THR:HG21	1.95	0.49
1:C:388:TYR:HE1	1:C:411:ALA:CA	2.26	0.49
1:C:425:LEU:O	1:C:429:HIS:HD2	1.96	0.49
1:G:439:ILE:HG23	1:G:459:LEU:HD11	1.95	0.49
1:G:723:ARG:HD2	1:G:829:GLU:O	2.13	0.49
1:G:376:GLU:O	1:G:380:ILE:HG12	2.12	0.48
1:G:1009:LEU:O	1:G:1013:MET:HG3	2.12	0.48
1:E:327:LYS:HA	1:E:327:LYS:CE	2.33	0.48
1:G:839:GLN:HB2	1:G:841:TYR:CE1	2.48	0.48
1:G:851:TRP:CD1	1:G:912:LEU:HD13	2.48	0.48
1:A:497:PRO:HB2	1:A:655:TYR:OH	2.13	0.48
1:C:822:ARG:NH2	1:C:909:ASP:OD1	2.46	0.48
1:E:439:ILE:HG23	1:E:459:LEU:HD11	1.95	0.48
1:E:480:VAL:HG22	1:E:505:LEU:HD23	1.96	0.48
1:E:708:LYS:HG2	1:E:988:TRP:CH2	2.48	0.48
1:G:933:MET:O	1:G:958:LEU:HB3	2.14	0.48
1:A:576:PHE:CE1	1:A:1007:GLU:HB3	2.48	0.48
1:C:667:ILE:O	1:C:667:ILE:HG23	2.12	0.48
1:E:410:ARG:HH12	1:G:410:ARG:HH12	1.61	0.48
1:E:685:LYS:HD2	1:E:1025:HIS:CE1	2.48	0.48
1:E:826:GLY:HA2	2:F:941:TYR:CD2	2.48	0.48
1:E:834:TYR:O	1:E:863:LEU:HD12	2.13	0.48
1:G:650:ALA:CB	1:G:666:TYR:HB2	2.43	0.48
1:G:723:ARG:HA	1:G:822:ARG:HG3	1.95	0.48
1:A:699:ALA:HA	1:A:928:TRP:CZ2	2.49	0.48
1:C:387:ALA:O	1:C:388:TYR:CG	2.67	0.48
1:C:651:MET:SD	1:C:664:MET:HG3	2.53	0.48
1:C:722:ASN:ND2	1:C:909:ASP:OD2	2.46	0.48
1:E:1019:ALA:HB3	1:E:1021:ASN:OD1	2.13	0.48
1:A:479:LEU:HA	1:A:482:ILE:HD12	1.96	0.48
1:C:466:VAL:HG12	1:C:871:VAL:CG2	2.43	0.48
1:E:854:ILE:CD1	1:E:967:GLU:HA	2.42	0.48
1:E:498:HIS:O	1:E:501:MET:HG2	2.13	0.48
1:E:713:PHE:O	1:E:769:MET:HE3	2.14	0.48



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:898:LYS:HZ3	3:G:1201:UD1:H1B	1.79	0.48
1:A:785:ILE:HG12	1:A:802:GLN:NE2	2.29	0.48
1:G:476:MET:HE1	1:G:503:TYR:HD1	1.79	0.48
1:G:937:PRO:HB2	1:G:944:ARG:HG2	1.95	0.48
1:A:426:ALA:HB3	1:A:442:TYR:CE1	2.49	0.48
1:C:327:LYS:HB3	1:C:332:ASN:HB3	1.95	0.48
1:E:367:LEU:HA	1:E:370:ALA:HB3	1.94	0.48
1:E:583:LEU:HD13	1:E:637:ARG:HB2	1.95	0.48
1:G:799:ALA:HA	2:H:937:PHE:HZ	1.79	0.48
1:G:841:TYR:OH	3:G:1201:UD1:C8'	2.62	0.48
1:A:738:LEU:HB2	1:A:741:VAL:CG2	2.44	0.47
1:A:886:PRO:HG2	1:A:889:ARG:HG2	1.96	0.47
1:C:419:ALA:HB1	1:C:445:ALA:O	2.14	0.47
1:E:818:ILE:HG21	1:E:903:ARG:CD	2.44	0.47
1:G:392:GLY:HA3	1:G:408:TYR:CE1	2.49	0.47
1:G:516:ARG:O	1:G:520:LEU:HG	2.14	0.47
1:G:596:MET:HA	1:G:602:PHE:CD2	2.48	0.47
1:E:453:PRO:HB3	1:E:482:ILE:HG21	1.97	0.47
1:A:367:LEU:HD23	1:A:367:LEU:H	1.79	0.47
1:A:442:TYR:CE2	1:A:458:ASN:HB3	2.48	0.47
1:A:469:TRP:CE3	1:A:845:PRO:HG3	2.49	0.47
1:C:356:ASN:O	1:C:360:VAL:HG12	2.15	0.47
1:C:466:VAL:HG12	1:C:871:VAL:HG21	1.96	0.47
1:E:523:ASP:HA	1:E:526:ASN:OD1	2.15	0.47
1:E:564:MET:HA	1:E:567:ILE:CD1	2.44	0.47
1:E:713:PHE:HA	1:E:769:MET:HE2	1.95	0.47
1:G:557:ASN:HB2	1:G:589:THR:HG21	1.96	0.47
1:G:563:LEU:HD22	1:G:696:GLY:HA2	1.97	0.47
1:G:675:PRO:O	1:G:678:VAL:HG22	2.14	0.47
1:G:692:THR:HA	1:G:948:SER:OG	2.14	0.47
1:A:821:THR:HG22	1:A:824:GLN:OE1	2.15	0.47
1:A:1025:HIS:HB3	1:A:1027:ILE:CD1	2.44	0.47
1:C:818:ILE:HG21	1:C:903:ARG:NE	2.30	0.47
1:C:855:LEU:HD12	1:C:861:SER:OG	2.14	0.47
1:E:658:THR:CB	1:E:682:TYR:HA	2.44	0.47
1:E:734:PHE:HE1	1:E:738:LEU:HD11	1.78	0.47
1:G:474:GLU:HA	1:G:477:LYS:HG2	1.96	0.47
1:A:426:ALA:HB3	1:A:442:TYR:CD1	2.49	0.47
1:A:685:LYS:HD2	1:A:1025:HIS:N	2.30	0.47
1:C:452:PHE:HD2	1:C:455:ALA:CB	2.27	0.47
1:C:553:SER:CB	1:C:583:LEU:HB2	2.43	0.47



	lo uo pago	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:698:HIS:CE1	1:A:924:MET:HB3	2.49	0.47
1:C:976:ASP:HB3	1:C:979:TYR:HB3	1.96	0.47
1:G:514:ALA:HB1	1:G:659:SER:O	2.13	0.47
1:A:350:PHE:CD2	1:A:353:ALA:HB2	2.49	0.47
1:A:879:TYR:O	1:A:883:MET:HG3	2.14	0.47
2:B:942:LEU:C	2:B:943:LEU:HD12	2.35	0.47
1:C:323:LEU:HA	1:C:326:ILE:HD12	1.97	0.47
1:C:839:GLN:HG2	1:C:868:PHE:HE2	1.70	0.47
1:G:799:ALA:HB2	2:H:937:PHE:CE2	2.50	0.47
1:E:728:GLY:HA3	1:E:817:ILE:HD13	1.96	0.47
1:G:342:LYS:O	1:G:342:LYS:HD3	2.14	0.47
1:G:1008:ARG:O	1:G:1012:GLN:HG3	2.15	0.47
1:A:552:SER:HA	1:A:630:ASN:OD1	2.15	0.47
1:C:471:ASP:HB3	1:C:474:GLU:OE2	2.15	0.47
1:C:650:ALA:CB	1:C:666:TYR:HB2	2.45	0.47
1:E:886:PRO:HB2	1:E:888:ASN:OD1	2.14	0.47
1:E:979:TYR:O	1:E:983:VAL:HG23	2.15	0.47
1:G:538:ASP:HB2	1:G:540:LYS:HD3	1.97	0.47
1:G:896:ALA:HB1	1:G:900:GLU:HB3	1.97	0.47
1:A:685:LYS:CE	1:A:1024:ASP:HA	2.45	0.47
1:C:349:GLU:HA	1:C:380:ILE:CD1	2.44	0.47
1:C:452:PHE:HD2	1:C:455:ALA:HB3	1.80	0.47
1:C:837:PHE:HD1	1:C:866:LEU:HD23	1.79	0.47
1:E:953:LEU:HB3	1:E:955:CYS:SG	2.54	0.47
1:A:823:SER:OG	2:B:943:LEU:HD11	2.15	0.46
1:E:374:TYR:HB3	1:E:391:MET:CE	2.38	0.46
1:E:554:ASP:HB3	1:E:558:HIS:CG	2.50	0.46
1:E:706:LYS:O	1:E:991:ARG:NH2	2.48	0.46
1:G:412:ILE:CD1	1:G:421:ALA:HB3	2.44	0.46
1:A:489:LYS:HB2	1:A:491:ARG:HG3	1.97	0.46
1:A:820:THR:HA	1:A:824:GLN:OE1	2.15	0.46
1:C:374:TYR:HB3	1:C:391:MET:HE2	1.97	0.46
1:C:395:LEU:HD12	1:C:407:CYS:SG	2.55	0.46
1:E:492:LEU:HD11	1:E:520:LEU:HD11	1.97	0.46
1:G:558:HIS:CG	1:G:559:PRO:HD2	2.49	0.46
1:G:920:HIS:O	1:G:921:THR:HB	2.15	0.46
3:G:1201:UD1:H1'	3:G:1201:UD1:O7'	2.15	0.46
1:A:474:GLU:OE1	1:A:474:GLU:N	2.36	0.46
1:C:497:PRO:HD3	1:C:517:HIS:NE2	2.30	0.46
1:E:626:LEU:HB3	1:E:649:GLN:HG2	1.97	0.46
1:C:834:TYR:HD2	1:C:912:LEU:HD21	1.79	0.46



	1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:850:MET:HE1	1:C:963:ARG:HA	1.97	0.46
1:E:856:LYS:HD3	1:E:885:LEU:HD21	1.98	0.46
1:A:533:TYR:CD2	1:A:645:PRO:HA	2.50	0.46
1:A:723:ARG:HA	1:A:822:ARG:HG3	1.98	0.46
1:A:723:ARG:HH21	1:A:829:GLU:HB3	1.80	0.46
1:G:546:LEU:CD1	1:G:624:HIS:HB2	2.46	0.46
1:A:366:LYS:HB3	1:A:369:GLU:CB	2.42	0.46
1:C:344:LEU:CD2	1:C:353:ALA:HB1	2.45	0.46
1:E:923:GLY:O	1:E:927:LEU:HD12	2.15	0.46
1:G:476:MET:O	1:G:480:VAL:HG23	2.15	0.46
1:G:797:GLY:HA3	1:G:903:ARG:HH12	1.80	0.46
1:A:566:SER:O	1:A:570:MET:HG3	2.16	0.46
1:C:388:TYR:HE1	1:C:411:ALA:N	2.13	0.46
1:C:582:ALA:HB2	1:C:602:PHE:CZ	2.50	0.46
1:C:855:LEU:HD23	1:C:885:LEU:CD1	2.46	0.46
1:E:410:ARG:NH1	1:G:410:ARG:HH22	2.14	0.46
1:E:484:ALA:O	1:E:488:GLU:HG2	2.16	0.46
1:E:786:GLN:HB2	1:E:794:ILE:O	2.15	0.46
1:E:988:TRP:O	1:E:991:ARG:HG2	2.16	0.46
1:A:492:LEU:HD13	1:A:520:LEU:HD21	1.98	0.46
1:A:779:MET:HE3	1:A:794:ILE:HG22	1.96	0.46
1:A:800:THR:CA	1:A:803:ILE:HG22	2.44	0.46
1:C:320:LEU:HB2	1:C:343:ALA:HB2	1.97	0.46
1:G:780:ILE:O	2:H:939:PRO:HD3	2.16	0.46
1:G:873:GLU:HG3	1:G:892:PHE:CD2	2.50	0.46
1:A:384:PHE:HD2	1:A:387:ALA:CB	2.29	0.46
1:A:675:PRO:HD2	1:A:678:VAL:CG1	2.46	0.46
1:C:328:ARG:O	1:C:328:ARG:NH1	2.38	0.46
1:C:552:SER:HA	1:C:630:ASN:OD1	2.15	0.46
1:E:347:PHE:HD1	1:E:348:PRO:HD2	1.81	0.46
1:E:937:PRO:HB2	1:E:944:ARG:NH1	2.31	0.46
1:G:723:ARG:NH1	1:G:829:GLU:OE1	2.49	0.46
1:G:769:MET:HE2	2:H:945:LEU:HB2	1.98	0.46
1:G:945:VAL:O	1:G:949:GLN:HG3	2.15	0.46
1:A:333:ILE:HA	1:A:336:ALA:HB3	1.98	0.46
1:A:525:ILE:HB	1:A:643:LEU:HD11	1.98	0.46
1:A:855:LEU:HB3	1:A:889:ARG:NH2	2.31	0.46
1:E:323:LEU:O	1:E:327:LYS:HG2	2.15	0.46
1:E:426:ALA:HB1	1:E:438:ALA:O	2.15	0.46
1:G:549:GLY:HA2	1:G:579:PHE:O	2.16	0.46
1:G:652:TRP:CG	1:G:653:LEU:N	2.84	0.46



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:822:ARG:HA	1:A:907:LEU:HD13	1.97	0.45	
1:C:911:CYS:HB2	1:C:926:VAL:HG21	1.97	0.45	
1:E:446:LEU:HD21	1:E:455:ALA:HB3	1.97	0.45	
1:E:923:GLY:C	1:E:927:LEU:HD12	2.36	0.45	
1:G:409:THR:O	1:G:413:GLN:HG3	2.16	0.45	
1:A:374:TYR:CD2	1:A:391:MET:HA	2.51	0.45	
1:E:808:ALA:HB1	1:E:897:PRO:HB3	1.98	0.45	
1:G:721:ASP:OD2	1:G:984:ARG:HD3	2.17	0.45	
1:G:787:ILE:HG13	1:G:794:ILE:HB	1.99	0.45	
1:G:797:GLY:HA3	1:G:903:ARG:NH1	2.31	0.45	
1:G:926:VAL:HG13	1:G:931:THR:HB	1.97	0.45	
1:A:521:CYS:HB2	1:A:639:GLU:HG3	1.97	0.45	
1:C:953:LEU:O	1:C:990:GLN:NE2	2.46	0.45	
1:E:838:ASN:HB3	1:E:842:LYS:HD2	1.99	0.45	
1:G:822:ARG:HH12	1:G:831:ALA:H	1.63	0.45	
1:A:496:HIS:CG	1:A:497:PRO:HD2	2.51	0.45	
1:C:673:THR:CG2	1:C:693:PHE:HE1	2.22	0.45	
1:E:452:PHE:HD2	1:E:455:ALA:HB3	1.80	0.45	
1:E:548:VAL:HG21	1:E:1010:TYR:CD2	2.51	0.45	
1:E:912:LEU:HB3	1:E:966:TYR:OH	2.17	0.45	
1:E:953:LEU:HG	1:E:990:GLN:HB3	1.97	0.45	
1:G:711:ILE:HG13	1:G:726:LEU:HD11	1.99	0.45	
1:G:960:ALA:HB1	1:G:965:GLU:HB3	1.99	0.45	
1:A:497:PRO:HD3	1:A:517:HIS:CE1	2.52	0.45	
1:A:521:CYS:HA	1:A:524:LYS:HD3	1.98	0.45	
1:C:516:ARG:HD2	1:C:516:ARG:N	2.31	0.45	
1:C:850:MET:HE1	1:C:966:TYR:HB3	1.98	0.45	
1:E:841:TYR:CZ	1:E:842:LYS:HE2	2.51	0.45	
1:E:953:LEU:HD13	1:E:996:LEU:HD22	1.98	0.45	
1:E:1003:THR:O	1:E:1007:GLU:HG3	2.16	0.45	
1:G:479:LEU:O	1:G:483:VAL:HG23	2.16	0.45	
1:A:327:LYS:HD2	1:A:332:ASN:HB3	1.99	0.45	
1:A:846:SER:HB2	1:A:963:ARG:HH12	1.81	0.45	
1:C:368:GLN:OE1	1:C:369:GLU:OE2	2.35	0.45	
1:C:535:HIS:ND1	1:C:647:PRO:HA	2.31	0.45	
1:E:780:ILE:O	2:F:939:PRO:HD3	2.17	0.45	
1:G:562:HIS:HE1	1:G:898:LYS:HE3	1.76	0.45	
1:A:350:PHE:CE1	1:A:352:ALA:HB3	2.52	0.45	
1:A:480:VAL:HG13	1:A:505:LEU:HD23	1.98	0.45	
2:D:942:LEU:H	2:D:942:LEU:CD2	2.23	0.45	
1:E:808:ALA:HB1	1:E:897:PRO:CB	2.46	0.45	



		Interatomic	Clash	
Atom-1	tom-1 Atom-2		overlap (Å)	
1:G:315:THR:OG1	1:G:316:HIS:N	2.47	0.45	
1:A:412:ILE:HG13	1:A:421:ALA:HB1	1.97	0.45	
1:E:412:ILE:HG12	1:E:421:ALA:HB3	1.99	0.45	
1:G:584:SER:O	1:G:592:ARG:NH1	2.50	0.45	
1:A:381:SER:OG	1:A:384:PHE:HB2	2.17	0.45	
1:A:446:LEU:HD21	1:A:455:ALA:HB3	1.99	0.45	
1:A:661:ALA:HB1	1:A:663:PHE:CE2	2.52	0.45	
1:A:898:LYS:NZ	3:A:1201:UD1:O3B	2.42	0.45	
1:A:945:VAL:HG12	1:A:946:ALA:N	2.32	0.45	
1:C:324:ALA:CA	1:C:339:LEU:HD12	2.45	0.45	
1:C:661:ALA:HB1	1:C:663:PHE:CE1	2.52	0.45	
1:E:720:TYR:HB3	1:E:723:ARG:HB2	1.98	0.45	
1:E:850:MET:HE1	1:E:966:TYR:HB3	1.98	0.45	
1:A:616:ASP:O	1:A:620:GLN:HG2	2.17	0.45	
1:G:405:LEU:HD11	1:G:425:LEU:CD1	2.47	0.45	
1:A:615:ALA:HB3	1:A:643:LEU:HD23	1.99	0.44	
1:C:333:ILE:O	1:C:337:VAL:HG23	2.17	0.44	
1:C:497:PRO:HD3	1:C:517:HIS:CD2	2.52	0.44	
1:C:720:TYR:CD2	1:C:723:ARG:CD	2.98	0.44	
1:E:324:ALA:N	1:E:339:LEU:HD23	2.32	0.44	
1:G:470:THR:O	1:G:475:ARG:NH2	2.50	0.44	
1:C:850:MET:CE	1:C:966:TYR:HB3	2.46	0.44	
1:E:344:LEU:HD21	1:E:353:ALA:HB1	1.97	0.44	
1:E:393:ASN:O	1:E:397:GLU:HG2	2.16	0.44	
1:G:871:VAL:O	1:G:874:PRO:HD2	2.17	0.44	
1:C:854:ILE:HG21	1:C:970:ALA:CB	2.47	0.44	
1:E:516:ARG:O	1:E:520:LEU:HG	2.16	0.44	
2:F:945:LEU:N	2:F:946:PRO:HD3	2.32	0.44	
1:G:928:TRP:O	1:G:991:ARG:NH1	2.49	0.44	
1:C:873:GLU:HG3	1:C:892:PHE:CE2	2.52	0.44	
1:G:489:LYS:HB2	1:G:491:ARG:HG3	1.99	0.44	
1:G:934:VAL:HG12	1:G:966:TYR:CE1	2.52	0.44	
1:A:644:ARG:HA	1:A:644:ARG:HD3	1.67	0.44	
1:G:476:MET:HE1	1:G:503:TYR:CD1	2.53	0.44	
1:G:873:GLU:N	1:G:874:PRO:HD2	2.33	0.44	
1:A:355:SER:O	1:A:374:TYR:HE1	2.00	0.44	
1:A:456:TYR:OH	1:A:475:ARG:HA	2.17	0.44	
1:C:720:TYR:CD2	1:C:723:ARG:HD2	2.52	0.44	
1:C:804:ASN:ND2	1:C:807:ALA:HB2	2.33	0.44	
2:D:937:PHE:O	2:D:937:PHE:CG	2.70	0.44	
1:E:698:HIS:HE1	1:E:924:MET:HB3	1.82	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:927:LEU:HG	1:E:933:MET:CE	2.45	0.44	
1:G:323:LEU:HG	1:G:339:LEU:HD21	2.00	0.44	
1:G:324:ALA:CA	1:G:339:LEU:HD22	2.47	0.44	
1:G:785:ILE:HG22	1:G:786:GLN:HG2	2.00	0.44	
1:A:770:ASN:O	1:A:774:GLU:HG3	2.18	0.44	
1:A:839:GLN:HB2	1:A:841:TYR:CD2	2.53	0.44	
1:C:415:ASN:ND2	1:C:418:PHE:HB2	2.33	0.44	
1:C:1012:GLN:HB3	1:C:1026:MET:HE2	1.97	0.44	
1:E:480:VAL:HG22	1:E:505:LEU:CD2	2.48	0.44	
1:E:667:ILE:HG23	1:E:667:ILE:O	2.17	0.44	
1:A:384:PHE:CD2	1:A:387:ALA:HB2	2.50	0.44	
1:A:552:SER:HB2	1:A:629:MET:HB2	2.00	0.44	
1:A:695:ILE:HD12	1:A:696:GLY:H	1.81	0.44	
1:C:842:LYS:HD3	1:C:917:CYS:HB3	1.99	0.44	
1:E:533:TYR:HD2	1:E:619:HIS:CG	2.35	0.44	
1:E:678:VAL:O	1:E:678:VAL:HG13	2.17	0.44	
1:G:366:LYS:HD2	1:G:366:LYS:HA	1.65	0.44	
1:G:369:GLU:HA	1:G:372:MET:HG2	1.99	0.44	
1:A:358:ALA:HB2	1:A:373:HIS:CB	2.40	0.44	
1:A:771:THR:HA	1:A:774:GLU:HG3	2.00	0.44	
1:C:480:VAL:HG22	1:C:505:LEU:CD2	2.48	0.44	
1:C:806:LYS:HA	1:C:806:LYS:HD3	1.63	0.44	
1:G:836:ASN:ND2	1:G:912:LEU:O	2.50	0.44	
1:A:367:LEU:HD12	1:A:398:MET:HG2	2.00	0.43	
1:C:724:ILE:HG23	1:C:821:THR:CG2	2.45	0.43	
1:C:725:VAL:HG12	1:C:820:THR:O	2.18	0.43	
1:C:772:ILE:O	1:C:776:VAL:HG23	2.18	0.43	
3:C:1201:UD1:H1'	3:C:1201:UD1:O1A	2.18	0.43	
1:E:614:ALA:HB3	1:E:640:LEU:HD21	2.00	0.43	
1:E:630:ASN:O	1:E:633:THR:OG1	2.31	0.43	
1:E:827:LEU:CD1	1:E:833:VAL:HG11	2.48	0.43	
1:E:921:THR:O	1:E:925:ASP:OD2	2.35	0.43	
1:C:720:TYR:HD2	1:C:723:ARG:HD2	1.81	0.43	
1:C:854:ILE:HG21	1:C:970:ALA:HB1	2.00	0.43	
1:C:937:PRO:HD2	1:C:960:ALA:O	2.18	0.43	
1:E:340:TYR:CE1	1:E:356:ASN:HB2	2.53	0.43	
1:E:793:SER:C	1:E:794:ILE:HD13	2.37	0.43	
1:G:670:ASP:OD1	1:G:671:GLN:O	2.36	0.43	
1:G:860:ASN:OD1	1:G:860:ASN:C	2.56	0.43	
1:A:821:THR:N	1:A:824:GLN:OE1	2.50	0.43	
1:A:1007:GLU:O	1:A:1011:LEU:HG	2.18	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:379:ARG:NH1	1:C:380:ILE:HG12	2.34	0.43	
1:E:357:LEU:HD12	1:E:360:VAL:CG2	2.49	0.43	
1:E:553:SER:CB	1:E:583:LEU:HB2	2.40	0.43	
1:E:672:GLU:OE2	1:E:951:THR:HG21	2.18	0.43	
1:G:725:VAL:CG1	1:G:820:THR:HB	2.46	0.43	
1:G:833:VAL:HG23	1:G:908:ALA:HA	2.00	0.43	
1:G:844:ASP:OD2	1:G:916:LEU:HD22	2.17	0.43	
1:A:720:TYR:HD2	1:A:723:ARG:HD3	1.83	0.43	
1:A:933:MET:CE	1:A:946:ALA:HB1	2.49	0.43	
1:C:463:LEU:HD22	1:C:468:ASP:HB3	2.00	0.43	
1:C:605:LEU:HA	1:C:608:ILE:CD1	2.37	0.43	
1:E:698:HIS:HE1	1:E:924:MET:CB	2.31	0.43	
1:G:519:ASN:HA	1:G:522:LEU:HD12	1.99	0.43	
1:G:901:HIS:CE1	1:G:922:THR:HG23	2.53	0.43	
1:A:967:GLU:O	1:A:971:VAL:HG23	2.18	0.43	
1:C:496:HIS:CG	1:C:497:PRO:HD2	2.54	0.43	
1:C:567:ILE:HD12	1:C:1003:THR:OG1	2.18	0.43	
1:E:439:ILE:HD13	1:E:463:LEU:HD23	2.00	0.43	
1:E:684:GLU:CD	1:E:684:GLU:H	2.21	0.43	
1:E:698:HIS:ND1	1:E:997:PHE:HE2	2.17	0.43	
1:G:374:TYR:HB3	1:G:391:MET:HG3	2.00	0.43	
1:A:710:VAL:HA	1:A:724:ILE:O	2.18	0.43	
1:A:500:SER:HB2	1:A:510:ARG:HD3	2.01	0.43	
1:A:821:THR:HG23	1:A:824:GLN:H	1.83	0.43	
1:C:461:HIS:O	1:C:465:ILE:HG13	2.19	0.43	
1:C:850:MET:CE	1:C:963:ARG:HA	2.49	0.43	
1:E:492:LEU:HD13	1:E:520:LEU:HD11	2.00	0.43	
1:E:866:LEU:HA	1:E:893:SER:O	2.19	0.43	
1:E:899:GLU:CD	1:E:903:ARG:HE	2.21	0.43	
1:G:408:TYR:CE2	1:G:428:ILE:HD11	2.53	0.43	
1:G:769:MET:CE	2:H:945:LEU:HB2	2.49	0.43	
2:H:941:TYR:HD1	2:H:942:LEU:O	2.02	0.43	
1:A:393:ASN:O	1:A:396:LYS:HB2	2.19	0.43	
1:A:631:GLY:HA3	1:A:655:TYR:HB2	2.01	0.43	
1:C:360:VAL:HG13	1:C:361:LEU:HD12	2.00	0.43	
1:C:368:GLN:C	1:C:370:ALA:H	2.21	0.43	
1:G:685:LYS:HD2	1:G:1025:HIS:N	2.34	0.43	
1:G:807:ALA:HA	1:G:812:GLU:O	2.19	0.43	
1:G:898:LYS:O	1:G:902:VAL:HG23	2.18	0.43	
1:A:463:LEU:HD13	1:A:475:ARG:NH2	2.33	0.43	
2:B:937:PHE:CG	2:B:937:PHE:O	2.72	0.43	



	A the C	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:366:LYS:HD2	1:E:366:LYS:HA	1.78	0.43	
1:E:366:LYS:HG3	1:E:369:GLU:HB3	2.01	0.43	
1:E:545:ARG:HD2	1:E:576:PHE:O	2.19	0.43	
1:E:933:MET:SD	1:E:933:MET:N	2.91	0.43	
1:G:546:LEU:HD11	1:G:624:HIS:HB2	1.99	0.43	
1:G:699:ALA:HA	1:G:928:TRP:CH2	2.54	0.43	
1:G:857:ARG:CZ	1:G:971:VAL:HG21	2.49	0.43	
1:A:426:ALA:HB1	1:A:438:ALA:O	2.19	0.43	
1:A:552:SER:HB3	1:A:555:PHE:CE2	2.53	0.43	
1:C:1016:HIS:CD2	1:C:1021:ASN:HB2	2.54	0.43	
1:E:666:TYR:HE2	1:E:1026:MET:HG2	1.84	0.43	
1:G:586:ASP:HA	1:G:592:ARG:CD	2.48	0.43	
1:A:682:TYR:CD2	1:A:686:LEU:HD21	2.54	0.42	
1:A:834:TYR:HD1	1:A:912:LEU:HD21	1.84	0.42	
1:C:699:ALA:HA	1:C:928:TRP:CH2	2.53	0.42	
1:E:318:ASP:OD1	1:E:322:ASN:ND2	2.52	0.42	
1:E:378:ILE:CD1	1:E:387:ALA:HB3	2.49	0.42	
1:E:497:PRO:HB2	1:E:655:TYR:OH	2.18	0.42	
1:E:686:LEU:HD23	1:E:686:LEU:HA	1.88	0.42	
3:E:1201:UD1:H2B	3:E:1201:UD1:H6	1.84	0.42	
1:A:895:VAL:HG13	3:A:1201:UD1:O4	2.19	0.42	
1:E:319:SER:O	1:E:323:LEU:HD23	2.19	0.42	
1:E:453:PRO:HB3	1:E:482:ILE:CG2	2.48	0.42	
1:G:372:MET:SD	1:G:372:MET:N	2.92	0.42	
1:G:841:TYR:OH	3:G:1201:UD1:H8'1	2.19	0.42	
1:G:898:LYS:NZ	3:G:1201:UD1:O3B	2.49	0.42	
1:G:955:CYS:HB3	1:G:958:LEU:HD12	2.01	0.42	
1:A:321:ASN:HD21	1:A:356:ASN:ND2	2.17	0.42	
1:C:350:PHE:CD1	1:C:353:ALA:HB2	2.54	0.42	
1:C:387:ALA:C	1:C:389:SER:H	2.22	0.42	
1:C:474:GLU:H	1:C:474:GLU:CD	2.22	0.42	
1:C:725:VAL:C	1:C:726:LEU:HD12	2.39	0.42	
1:E:734:PHE:HD2	1:E:792:PHE:CB	2.31	0.42	
1:G:631:GLY:HA3	1:G:655:TYR:HB2	2.01	0.42	
1:G:695:ILE:HG13	1:G:696:GLY:N	2.34	0.42	
1:A:823:SER:HB3	2:B:943:LEU:HD11	1.99	0.42	
1:C:326:ILE:HG13	1:C:326:ILE:H	1.62	0.42	
1:C:665:ASP:HB3	1:C:1023:PRO:CG	2.49	0.42	
1:C:795:SER:HB2	1:C:803:ILE:CD1	2.49	0.42	
1:E:326:ILE:HD12	1:E:326:ILE:HA	1.88	0.42	
1:E:357:LEU:HD23	1:E:373:HIS:CD2	2.54	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:1012:GLN:HB2	1:G:1026:MET:CE	2.50	0.42	
1:A:405:LEU:HD13	1:A:428:ILE:HD12	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		
1:C:357:LEU:HA	1:C:360:VAL:HG12	2.01	0.42	
1:E:471:ASP:HA	1:E:474:GLU:OE2	2.20	0.42	
1:G:704:HIS:HB3	1:G:729:ILE:HD11	2.01	0.42	
1:G:937:PRO:HB3	1:G:944:ARG:HA	2.01	0.42	
2:H:943:LEU:O	2:H:943:LEU:HD12	2.20	0.42	
1:A:327:LYS:HD2	1:A:332:ASN:CB	2.49	0.42	
1:A:679:ALA:O	1:A:680:GLU:HB2	2.20	0.42	
1:E:429:HIS:CE1	1:E:437:GLU:HG2	2.54	0.42	
1:E:653:LEU:HB3	1:E:654:GLY:H	1.54	0.42	
1:A:945:VAL:C	1:A:947:ALA:H	2.22	0.42	
1:C:349:GLU:CA	1:C:380:ILE:HD13	2.48	0.42	
1:C:449:LYS:O	1:C:452:PHE:HB2	2.20	0.42	
1:C:928:TRP:O	1:C:991:ARG:NH1	2.51	0.42	
1:E:566:SER:OG	1:E:697:ASP:OD1	2.34	0.42	
1:E:738:LEU:HB2	1:E:741:VAL:HG23	2.01	0.42	
1:G:698:HIS:NE2	1:G:925:ASP:OD1	2.37	0.42	
1:G:920:HIS:O	3:G:1201:UD1:PB	2.78	0.42	
1:A:342:LYS:O	1:A:346:VAL:HG23	2.20	0.42	
1:A:719:ILE:CG2	1:A:744:VAL:HG11	2.50	0.42	
1:A:825:TYR:CZ	1:A:904:ARG:HG2	2.55	0.42	
1:G:472:TYR:O	1:G:476:MET:HG2	2.20	0.42	
1:G:787:ILE:CG1	1:G:794:ILE:HB	2.50	0.42	
1:A:690:PRO:HG2	1:A:1005:GLU:OE1	2.19	0.42	
1:C:723:ARG:O	1:C:724:ILE:C	2.58	0.42	
1:E:350:PHE:HE1	1:E:352:ALA:HB3	1.83	0.42	
1:E:422:HIS:HB2	1:E:445:ALA:HB2	2.01	0.42	
1:E:678:VAL:HG21	1:E:681:GLN:HE21	1.81	0.42	
1:E:795:SER:HB3	1:E:803:ILE:HD13	2.01	0.42	
1:G:667:ILE:HG22	1:G:684:GLU:HB2	2.02	0.42	
1:G:804:ASN:OD1	1:G:806:LYS:HB2	2.19	0.42	
1:A:854:ILE:HD13	1:A:971:VAL:HG23	2.02	0.42	
1:E:358:ALA:HB2	1:E:373:HIS:HB2	2.01	0.42	
1:E:726:LEU:CG	1:E:819:VAL:HG22	2.48	0.42	
1:E:896:ALA:HB1	1:E:900:GLU:HB3	2.01	0.42	
1:E:1007:GLU:O	1:E:1011:LEU:HG	2.19	0.42	
1:G:497:PRO:HD3	1:G:517:HIS:CE1	2.55	0.42	
1:G:723:ARG:NH1	1:G:830:ASP:HB3	2.35	0.42	
1:A:324:ALA:HB1	1:A:340:TYR:CD2	2.55	0.41	
1:A:565:GLN:NE2	1:A:697:ASP:OD2	2.43	0.41	



	A	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:360:VAL:O	1:C:364:GLN:N	2.45	0.41	
1:E:340:TYR:CB	1:E:357:LEU:HD13	U:HD13 2.49		
1:E:645:PRO:HD2	1:E:649:GLN:OE1	2.19	0.41	
1:G:685:LYS:HD2	1:G:1024:ASP:HA	2.01	0.41	
1:A:688:TYR:O	1:A:1009:LEU:HD22	2.20	0.41	
1:A:867:ARG:HB3	1:A:870:ALA:HA	2.02	0.41	
1:E:358:ALA:HB2	1:E:373:HIS:CB	2.50	0.41	
1:G:565:GLN:HE22	1:G:591:PHE:HD1	1.68	0.41	
1:G:797:GLY:HA2	1:G:818:ILE:CG2	2.49	0.41	
1:A:318:ASP:C	1:A:318:ASP:OD1	2.59	0.41	
1:A:332:ASN:O	1:A:336:ALA:N	2.53	0.41	
1:A:446:LEU:CD2	1:A:455:ALA:HB3	2.50	0.41	
1:C:461:HIS:CE1	1:C:465:ILE:HD11	2.56	0.41	
1:E:698:HIS:CE1	1:E:924:MET:HB3	2.55	0.41	
1:G:349:GLU:HB3	1:G:380:ILE:HD12	2.02	0.41	
1:A:946:ALA:O	1:A:950:LEU:HD13	2.20	0.41	
1:E:580:CYS:HB2	1:E:602:PHE:CD1	2.54	0.41	
1:E:714:LYS:HZ1	2:F:946:PRO:CB	2.33	0.41	
1:E:818:ILE:CG2	1:E:903:ARG:HD2	2.49	0.41	
1:G:387:ALA:HA	1:G:390:ASN:OD1	2.19	0.41	
1:G:567:ILE:HB	1:G:568:PRO:HD3	2.02	0.41	
1:C:342:LYS:HA	1:C:342:LYS:HD2	1.84	0.41	
1:C:885:LEU:HD23	1:C:885:LEU:HA	1.81	0.41	
1:E:780:ILE:O	2:F:939:PRO:HG3	2.21	0.41	
1:E:824:GLN:H	1:E:824:GLN:HG3	1.68	0.41	
1:G:782:ARG:HE	1:G:782:ARG:HB3	1.77	0.41	
1:G:687:ALA:O	1:G:1009:LEU:HD21	2.20	0.41	
1:G:697:ASP:O	1:G:701:MET:HG3	2.20	0.41	
1:A:452:PHE:HD2	1:A:455:ALA:CB	2.32	0.41	
1:A:502:LEU:HD11	1:A:841:TYR:HD1	1.80	0.41	
1:C:581:TYR:CE1	1:C:603:ILE:HD13	2.55	0.41	
1:C:839:GLN:HB2	1:C:841:TYR:CD1	2.55	0.41	
1:C:961:LYS:HG3	1:C:965:GLU:OE1	2.21	0.41	
1:G:439:ILE:HG23	1:G:459:LEU:CD1	2.51	0.41	
1:A:461:HIS:CE1	1:A:465:ILE:HD11	2.56	0.41	
1:C:501:MET:HG3	1:C:502:LEU:HG	2.02	0.41	
1:C:522:LEU:HD21	1:C:663:PHE:HE1	1.83	0.41	
1:C:689:MET:HE1	1:C:1002:TYR:CE2	2.54	0.41	
1:C:850:MET:HE2	1:C:966:TYR:CD2	2.56	0.41	
1:E:804:ASN:HD22	1:E:807:ALA:HB2	1.84	0.41	
1:G:946:ALA:HA	1:G:949:GLN:HG3	2.03	0.41	



	1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:367:LEU:HD23	1:A:367:LEU:N	2.35	0.41	
1:A:564:MET:HE2	1:A:564:MET:HB2	1.88	0.41	
1:A:679:ALA:C	1:A:681:GLN:H	2.24	0.41	
1:C:561:SER:O	1:C:565:GLN:HB3	2.21	0.41	
1:E:351:ALA:HB2	1:E:380:ILE:HB	2.03	0.41	
1:E:422:HIS:CB	1:E:445:ALA:HB2	2.50	0.41	
1:E:536:PRO:HB3	1:E:541:LEU:HD21	2.02	0.41	
1:E:879:TYR:O	1:E:883:MET:HG3	2.21	0.41	
1:G:596:MET:HE3	1:G:602:PHE:CE1	2.56	0.41	
2:B:942:LEU:N	2:B:942:LEU:HD22	2.36	0.41	
1:E:410:ARG:O	1:E:414:ILE:HD12	2.21	0.41	
1:E:828:PRO:HB2	1:E:831:ALA:HB3	2.02	0.41	
1:G:434:ASN:OD1	1:G:437:GLU:HB2	2.21	0.41	
1:G:589:THR:HA	1:G:811:GLU:OE2	2.21	0.41	
1:G:855:LEU:HB3	1:G:889:ARG:NH2	2.36	0.41	
1:G:866:LEU:HA	1:G:893:SER:O	2.21	0.41	
1:A:711:ILE:HG12	1:A:767:ILE:HB	2.03	0.40	
1:A:773:ALA:O	1:A:777:ILE:HG13	2.21	0.40	
1:C:740:ASP:HB2	1:C:768:PRO:HG3	2.03	0.40	
1:E:537:LYS:HD2	1:E:1017:TYR:OH	2.21	0.40	
1:E:590:ASN:O	1:E:594:LYS:HG3	2.20	0.40	
1:E:714:LYS:HB3	1:E:769:MET:HG3	2.03	0.40	
2:F:938:SER:HB2	2:F:939:PRO:CD	2.43	0.40	
1:G:833:VAL:HG23	1:G:909:ASP:N	2.37	0.40	
1:A:324:ALA:HB1	1:A:340:TYR:CE2	2.56	0.40	
2:B:938:SER:CB	2:B:939:PRO:CD	2.99	0.40	
1:C:999:THR:OG1	1:C:1000:LYS:N	2.54	0.40	
1:E:398:MET:O	1:E:399:GLN:HB2	2.21	0.40	
1:E:537:LYS:HD2	1:E:1017:TYR:CZ	2.56	0.40	
1:G:320:LEU:CD1	1:G:342:LYS:HG3	2.46	0.40	
1:E:837:PHE:O	1:E:922:THR:HG21	2.21	0.40	
1:G:324:ALA:HB3	1:G:340:TYR:CE1	2.56	0.40	
1:G:328:ARG:NH1	1:G:363:GLN:OE1	2.54	0.40	
1:C:362:GLN:HG3	1:C:394:THR:HG23	2.02	0.40	
1:C:426:ALA:HB1	1:C:442:TYR:CD2	2.56	0.40	
1:E:911:CYS:HB3	1:E:933:MET:HB3	2.02	0.40	
1:G:986:LYS:O	1:G:990:GLN:HG2	2.21	0.40	
1:C:422:HIS:HB2	1:C:445:ALA:HB2	2.04	0.40	
1:C:689:MET:HE3	1:C:689:MET:HB3	1.96	0.40	
1:E:738:LEU:HD12	1:E:767:ILE:HD11	2.03	0.40	
1:G:327:LYS:O	1:G:331:GLY:HA3	2.21	0.40	



Atom-1	tom-1 Atom-2		Clash overlap (Å)
1:G:328:ARG:NH2	1:G:360:VAL:HA	2.37	0.40
1:G:412:ILE:HD11	1:G:421:ALA:CB	2.52	0.40
1:G:577:GLU:OE2	1:G:601:HIS:NE2	2.55	0.40
1:G:868:PHE:HB2	1:G:895:VAL:HG12	2.03	0.40
1:G:1016:HIS:O	1:G:1021:ASN:HB2	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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	689/723~(95%)	664 (96%)	24 (4%)	1 (0%)	51	83
1	С	689/723~(95%)	662 (96%)	26 (4%)	1 (0%)	51	83
1	Е	689/723~(95%)	658~(96%)	31 (4%)	0	100	100
1	G	689/723~(95%)	653~(95%)	34~(5%)	2(0%)	41	74
2	В	9/13~(69%)	8 (89%)	1 (11%)	0	100	100
2	D	9/13~(69%)	9 (100%)	0	0	100	100
2	F	9/13~(69%)	5~(56%)	4 (44%)	0	100	100
2	Н	9/13~(69%)	8 (89%)	1 (11%)	0	100	100
All	All	2792/2944~(95%)	2667 (96%)	121 (4%)	4 (0%)	51	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	364	GLN
1	G	921	THR
1	С	351	ALA
1	G	690	PRO



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	597/618~(97%)	589~(99%)	8 (1%)	69	83
1	С	597/618~(97%)	592~(99%)	5 (1%)	81	89
1	Ε	597/618~(97%)	591~(99%)	6 (1%)	76	86
1	G	597/618~(97%)	588~(98%)	9 (2%)	65	81
2	В	10/12~(83%)	10 (100%)	0	100	100
2	D	10/12~(83%)	10 (100%)	0	100	100
2	F	10/12~(83%)	10 (100%)	0	100	100
2	Н	10/12~(83%)	10 (100%)	0	100	100
All	All	2428/2520 (96%)	2400 (99%)	28 (1%)	71	84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	328	ARG
1	А	338	ARG
1	А	341	ARG
1	А	386	ASP
1	А	523	ASP
1	А	564	MET
1	А	617	ARG
1	А	671	GLN
1	С	379	ARG
1	С	384	PHE
1	С	689	MET
1	С	898	LYS
1	С	925	ASP
1	Е	350	PHE
1	Е	363	GLN
1	Е	368	GLN
1	Е	376	GLU
1	Е	384	PHE
1	Е	389	SER



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Mol	Chain	\mathbf{Res}	Type
1	G	350	PHE
1	G	515	GLU
1	G	594	LYS
1	G	617	ARG
1	G	651	MET
1	G	694	PHE
1	G	920	HIS
1	G	949	GLN
1	G	963	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	321	ASN
1	А	332	ASN
1	А	373	HIS
1	А	802	GLN
1	А	836	ASN
1	А	920	HIS
1	С	332	ASN
1	С	354	HIS
1	С	373	HIS
1	С	393	ASN
1	С	498	HIS
1	С	590	ASN
1	С	649	GLN
1	Е	681	GLN
1	G	364	GLN
1	G	557	ASN
1	G	918	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Cha	Chain	Chain Dea	Tiple	Bond lengths			Bond angles		
	туре	Unann	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UD1	А	1201	-	38,41,41	0.33	0	57,62,62	0.66	2 (3%)
3	UD1	Е	1201	-	38,41,41	0.34	0	57,62,62	0.67	2 (3%)
3	UD1	С	1201	-	38,41,41	0.34	0	57,62,62	0.67	2 (3%)
3	UD1	G	1201	-	38,41,41	0.39	0	57,62,62	0.71	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UD1	А	1201	-	-	8/26/63/63	0/3/3/3
3	UD1	Е	1201	-	-	15/26/63/63	0/3/3/3
3	UD1	С	1201	-	-	7/26/63/63	0/3/3/3
3	UD1	G	1201	-	-	13/26/63/63	0/3/3/3

There are no bond length outliers.

All	(8)	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	Е	1201	UD1	PB-01'-C1'	-3.54	106.05	119.74
3	С	1201	UD1	PB-01'-C1'	-3.51	106.19	119.74
3	А	1201	UD1	PB-01'-C1'	-3.34	106.83	119.74
3	G	1201	UD1	O3A-PB-O1'	3.25	109.03	102.48



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	С	1201	UD1	O3A-PB-O1'	2.95	108.44	102.48
3	А	1201	UD1	O3A-PB-O1'	2.94	108.42	102.48
3	Е	1201	UD1	O3A-PB-O1'	2.81	108.14	102.48
3	G	1201	UD1	PB-01'-C1'	-2.78	108.99	119.74

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	1201	UD1	O5'-C1'-O1'-PB
3	Е	1201	UD1	C5B-O5B-PA-O1A
3	Е	1201	UD1	C5B-O5B-PA-O2A
3	G	1201	UD1	C1'-C2'-N2'-C7'
3	G	1201	UD1	C1'-O1'-PB-O3A
3	G	1201	UD1	C1'-O1'-PB-O1B
3	G	1201	UD1	C5B-O5B-PA-O1A
3	G	1201	UD1	C5B-O5B-PA-O2A
3	А	1201	UD1	C3B-C4B-C5B-O5B
3	А	1201	UD1	O4B-C4B-C5B-O5B
3	С	1201	UD1	O4B-C4B-C5B-O5B
3	G	1201	UD1	C3B-C4B-C5B-O5B
3	G	1201	UD1	O4B-C4B-C5B-O5B
3	А	1201	UD1	C1'-O1'-PB-O3A
3	Е	1201	UD1	C8'-C7'-N2'-C2'
3	Е	1201	UD1	O7'-C7'-N2'-C2'
3	С	1201	UD1	C3B-C4B-C5B-O5B
3	Ε	1201	UD1	C2B-C1B-N1-C6
3	Ε	1201	UD1	C2B-C1B-N1-C2
3	Е	1201	UD1	C4'-C5'-C6'-O6'
3	G	1201	UD1	PB-O3A-PA-O5B
3	G	1201	UD1	C3'-C2'-N2'-C7'
3	Е	1201	UD1	O4B-C1B-N1-C2
3	Ε	1201	UD1	C5B-O5B-PA-O3A
3	Ε	1201	UD1	O4B-C1B-N1-C6
3	G	1201	UD1	PA-O3A-PB-O2B
3	А	1201	UD1	C4'-C5'-C6'-O6'
3	Е	1201	UD1	O5'-C5'-C6'-O6'
3	C	1201	UD1	C2B-C1B-N1-C6
3	E	1201	UD1	O5'-C1'-O1'-PB
3	Е	1201	UD1	PA-O3A-PB-O1B
3	G	$12\overline{01}$	UD1	PB-O3A-PA-O1A
3	G	1201	UD1	C1'-O1'-PB-O2B



		1	1 0	
Mol	Chain	\mathbf{Res}	Type	Atoms
3	С	1201	UD1	O4B-C1B-N1-C6
3	Е	1201	UD1	PA-O3A-PB-O2B
3	G	1201	UD1	C5B-O5B-PA-O3A
3	С	1201	UD1	O4B-C1B-N1-C2
3	Е	1201	UD1	O4B-C4B-C5B-O5B
3	А	1201	UD1	PA-O3A-PB-O2B
3	А	1201	UD1	O4B-C1B-N1-C6
3	А	1201	UD1	C2B-C1B-N1-C6
3	С	1201	UD1	C2B-C1B-N1-C2
3	А	1201	UD1	O5'-C5'-C6'-O6'

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1201	UD1	6	0
3	Е	1201	UD1	2	0
3	С	1201	UD1	3	0
3	G	1201	UD1	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	695/723~(96%)	0.03	7 (1%) 82 73	85, 121, 173, 217	1 (0%)
1	С	695/723~(96%)	0.04	10 (1%) 75 64	89, 125, 180, 215	1 (0%)
1	Ε	695/723~(96%)	0.07	17 (2%) 59 47	102, 146, 180, 218	1 (0%)
1	G	695/723~(96%)	0.03	9 (1%) 77 67	90, 127, 180, 217	1 (0%)
2	В	11/13~(84%)	-0.01	0 100 100	110, 123, 186, 188	0
2	D	11/13~(84%)	0.36	0 100 100	141, 145, 193, 199	0
2	F	11/13~(84%)	0.35	2(18%) 1 1	134, 158, 195, 213	0
2	Н	11/13~(84%)	0.29	1 (9%) 9 7	103, 130, 185, 203	0
All	All	2824/2944~(95%)	0.04	46 (1%) 72 61	85, 131, 179, 218	4 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	365	GLY	3.9
1	С	367	LEU	3.4
1	G	364	GLN	3.4
1	С	388	TYR	3.3
1	Е	719	ILE	3.1
1	Е	536	PRO	3.0
1	G	340	TYR	2.9
1	Е	340	TYR	2.9
1	Е	745	LYS	2.8
1	С	364	GLN	2.7
1	Е	414	ILE	2.6
1	С	373	HIS	2.6
1	А	1014	TRP	2.6
1	Е	973	LEU	2.6
1	A	769	MET	2.5
2	F	936	ALA	2.5



Mol	Chain	Res	Type	RSRZ
1	С	330	GLN	2.5
1	Е	364	GLN	2.4
1	Е	854 ILE		2.4
1	А	1017 TYR		2.4
1	Е	711	ILE	2.4
1	А	781	ASN	2.4
1	А	744	VAL	2.4
1	G	672	GLU	2.4
1	G	742	LYS	2.4
1	Е	746	MET	2.3
1	Е	388	TYR	2.3
1	Е	398	MET	2.3
1	Е	537	LYS	2.3
2	Н	946	PRO	2.3
1	С	369	GLU	2.3
1	Е	974	GLY	2.3
2	F	946	PRO	2.3
1	С	337	VAL	2.2
1	G	530	LYS	2.2
1	Е	1014	TRP	2.2
1	С	419	ALA	2.2
1	G	321	ASN	2.2
1	G	746	MET	2.1
1	А	640	LEU	2.1
1	С	829	GLU	2.1
1	Е	686	LEU	2.1
1	G	769	MET	2.1
1	G	645	PRO	2.1
1	С	885	LEU	2.1
1	Е	429	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UD1	Е	1201	39/39	0.91	0.31	109,153,236,247	10
3	UD1	С	1201	39/39	0.92	0.35	85,123,179,185	6
3	UD1	G	1201	39/39	0.92	0.31	91,143,223,251	9
3	UD1	А	1201	39/39	0.95	0.31	87,114,178,183	9

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











6.5 Other polymers (i)

There are no such residues in this entry.

