

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 31, 2020 - 09:37 AM BST

PDB ID	:	1DU3
Title	:	Crystal structure of TRAIL-SDR5
Authors	:	Cha, SS.; Sung, BJ.; Oh, BH.
Deposited on	:	2000-01-14
Resolution	:	2.20  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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
$\mathrm{EDS}$	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5594(2.20-2.20)
Ramachandran outliers	138981	5503(2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	130	25%	36%	8%	31%		
1	В	130	34%		39%	12% 15%		
1	С	130	18%	38%	12% •	31%		
1	G	130	33%		40%	10% 17%		
1	Н	130	28%	31%	10% •	31%		
1	Ι	130	22%	34%	12% •	31%		
2	D	168	46%		39%	5% • 10%		
2	Е	168	40%		39%	9% • 10%		



Mol	Chain	Length	Quality of chain				
2	F	168	36%	48%	7% 10%		
2	J	168	45%	40%	• • 10%		
2	K	168	43%	40%	5% • 10%		
2	L	168	36%	45%	10% 10%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	Ε	1	-	-	Х	-



#### $1\mathrm{DU3}$

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12108 atoms, of which 0 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.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace	
1	Δ	00	Total	С	Ν	Ο	S	0	0	0	
	Л	90	701	419	122	148	12	0	0	0	
1	В	110	Total	С	Ν	Ο	S	0	0	0	
	D	110	833	497	148	172	16	0	0	U	
1	С	00	Total	С	Ν	Ο	S	0	0	0	
		90	697	417	121	147	12	0		0	
1	С	108	Total	С	Ν	Ο	S	0	0	0	
	G	100	833	498	150	169	16	0	0	0	
1	ц	00	Total	С	Ν	Ο	S	0	0	0	
	11	90	691	414	118	147	12	0	0	0	
1	т	00	Total	С	Ν	Ο	S	0	0	0	
		90	701	419	122	148	12		U	U	

• Molecule 1 is a protein called DEATH RECEPTOR 5.

• Molecule 2 is a protein called TNF-RELATED APOPTOSIS INDUCING LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	п	159	Total	С	Ν	Ο	S	0	0	Ο
	D	102	1252	797	217	234	4	0	0	0
2	F	159	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	Ľ	102	1252	797	217	234	4	0	0	0
2	F	159	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	Ľ	102	1246	794	214	234	4	0	0	0
2	Т	159	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	ป	102	1248	795	217	232	4	0	0 0	0
9	K	159	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	IX	152	1252	797	217	234	4	0	0	0
2	Т	159	Total	C	Ν	Ō	S	0	0	0
	L	102	1238	789	212	233	4	0		0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Zn 1 1	0	0
3	Е	1	Total Zn 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	26	Total         O           26         26	0	0
4	В	23	TotalO2323	0	0
4	С	6	Total O 6 6	0	0
4	D	22	TotalO2222	0	0
4	Е	14	Total         O           14         14	0	0
4	F	13	Total         O           13         13	0	0
4	G	16	Total         O           16         16	0	0
4	Н	7	Total O 7 7	0	0
4	Ι	11	Total O 11 11	0	0
4	J	8	Total O 8 8	0	0
4	K	9	Total O 9 9	0	0
4	L	7	Total O 7 7	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: DEATH RECEPTOR 5

Chain A:	25%	36%	8%	31%	_
ALA LEU THR GIN GIN ASP ALA PRO	G GLN G GLN ALA ALA ALA C	S24 E25 G26 C28 P20 P20 B31 H32 H33 H33	L34 B335 D40 D40 C41 C41 C44 C44	K45 Y46 Q47 Q48 Y50 Y50 S51 T52	M54 M54 N55 L57 L58 F59 C60 L61
R62 C63 T64 T64 R65 C66 C66 G69 C69 C71	L72 L73 274 775 775 177 178 179 180 181 182 182 085	C86 E87 E87 E87 F91 R92 S96 F97 E98	C100 C100 K102 CYS CYS CYS ARG ARG CYS CYS CYS	ARG GLY MET MET VAL LYS CLY GLY G116	1118 1119 1119 1120 1123 1123 0120 0100 0100
VAL HIS LYS GLU SER					
• Molecule 1:	DEATH RECEP	TOR 5			
Chain B:	34%	39%	ó	12% 15	%
ALA LEU THE THR GLN GLN ASP ALA ALA PRO	GLN GLN ALA ALA ALA ALA CLN GLN GLN GLN GLN S2 1 S2 S2 S2 S2	S24 E25 626 626 729 P30 P30 P33 831 F33 F33	154 153 133 133 133 133 133 144 144 148	<b>P49</b> <b>Y50</b> <b>152</b> H53 H53 N55 D56	L58 F59 C60 L61 164 R65
S68 E72 E73 E74 E73 E74 E77 T78 T78 T79	N81 182 192 190 193 193 193 190 100	R101 R104 R104 G105 G105 R106 R109 R110 M111	V112 V114 V114 G115 G115 C117 T118 V119 W120 V120 V120	D122 1123 E124 C125 V126 K128 K128 E129	2
• Molecule 1:	DEATH RECEP	TOR 5			
Chain C:	18%	38%	12% •	31%	_
ALA LEU THR THR GLN GLN ASP ALA ALA ALA	6LN 6LN 6LN ALA ALA ALA ALA 6LN 6LN 6LN 6LN 521 521 522 523	に (131) (13	102 (102 (102 (102 (102 (102 (102 (102 (	D49 251 152 153 153 153 153 153	157 158 158 160 161 163 163 163
R65 066 066 868 874 173 874 875	C76 177 177 179 179 180 182 182 182 188 188 188 190 190	F91 F92 E93 E94 F97 F97 F97 F99 F99 F99 F99 F99	ALOL K102 CYS GLY CYS PRO ARG GLY GLY	MET VAL LYS VAL GLY GLY C117 T118	4120 8121 1123 6LU CYS VAL HIS
LYS GLU SER					
• Molecule 1:	DEATH RECEP	TOR 5			
Chain G:	33%	40%	5	10% 179	6
		W_O	RLDWIDE		

• PDB



![](_page_7_Picture_3.jpeg)

• Molecule 2: TNF-RELATED APOPTOSIS INDUCING LIGAND

![](_page_7_Figure_5.jpeg)

![](_page_7_Picture_6.jpeg)

#### 

#### 

![](_page_8_Picture_5.jpeg)

## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	68.63Å 124.81Å 128.37Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $104.49^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	8.00 - 2.20	Depositor	
% Data completeness	(Not available) $(8.00-2.20)$	Depositor	
(in resolution range)	(100 available) (0.00 2.20)	Depositor	
$R_{merge}$	0.06	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR 3.851	Depositor	
$R, R_{free}$	0.291 , $0.291$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	12108	wwPDB-VP	
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP	

![](_page_9_Picture_6.jpeg)

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mal	Mol Chain		nd lengths	Bo	ond angles
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.56	0/716	0.82	0/969
1	В	2.32	1/849~(0.1%)	1.89	2/1149~(0.2%)
1	С	0.51	0/712	0.72	0/964
1	G	0.62	0/851	0.80	0/1150
1	Н	0.58	0/706	0.79	0/957
1	Ι	0.98	1/716~(0.1%)	1.35	3/969~(0.3%)
2	D	0.86	5/1282~(0.4%)	0.81	1/1724~(0.1%)
2	Е	0.61	0/1282	0.79	0/1724
2	F	0.69	1/1276~(0.1%)	0.82	0/1717
2	J	0.62	0/1278	0.78	0/1719
2	Κ	0.61	0/1282	0.78	0/1724
2	L	0.64	0/1268	0.82	0/1708
All	All	0.89	8/12218~(0.1%)	0.95	6/16474~(0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

				_			
All (	(8)	bond	length	outliers	are	listed	below
* T T T	$( \cup )$	oona	10mS cm	outiful	aro	110000	5010.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	130	SER	C-O	-64.68	0.00	1.23
1	Ι	117	CYS	C-N	21.03	1.82	1.34
2	D	198	GLU	CG-CD	13.28	1.71	1.51
2	D	198	GLU	CD-OE1	9.92	1.36	1.25
2	F	191	ARG	C-N	-9.60	1.11	1.34
2	D	198	GLU	CD-OE2	6.92	1.33	1.25

![](_page_10_Picture_13.jpeg)

Continued from previous page							
$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type	Atoms	Z	0	

$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	D	191	ARG	C-N	-5.96	1.20	1.34
2	D	194	GLU	CB-CG	-5.29	1.42	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	130	SER	CA-C-O	-57.19	0.00	120.10
1	Ι	117	CYS	O-C-N	-25.30	82.22	122.70
1	Ι	117	CYS	C-N-CA	17.40	165.20	121.70
1	Ι	117	CYS	CA-C-N	17.17	154.98	117.20
1	В	127	HIS	O-C-N	-5.34	114.15	122.70
2	D	198	GLU	N-CA-C	5.22	125.10	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Group
2	F	205	GLN	Mainchain

## 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	701	0	619	46	0
1	В	833	0	735	75	1
1	С	697	0	613	94	0
1	G	833	0	755	63	0
1	Н	691	0	602	55	0
1	Ι	701	0	618	65	0
2	D	1252	0	1197	80	0
2	Е	1252	0	1200	81	0
2	F	1246	0	1188	99	0
2	J	1248	0	1196	73	0
2	K	1252	0	1200	75	0
2	L	1238	0	1172	105	0
3	Е	1	0	0	2	0
3	K	1	0	0	1	0

![](_page_11_Picture_14.jpeg)

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	26	0	0	0	0
4	В	23	0	0	3	2
4	С	6	0	0	2	0
4	D	22	0	0	7	0
4	Ε	14	0	0	2	0
4	F	13	0	0	2	0
4	G	16	0	0	0	1
4	Н	7	0	0	0	3
4	Ι	11	0	0	1	1
4	J	8	0	0	0	0
4	Κ	9	0	0	1	0
4	L	7	0	0	2	0
All	All	12108	0	11095	772	4

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 34.

All (772) 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:I:117:CYS:C	1:I:118:THR:N	1.82	1.33
1:C:75:PRO:HB3	2:L:170:ARG:HD3	1.30	1.13
1:B:58:LEU:HD23	4:B:3147:HOH:O	1.59	1.02
2:K:202:ASN:HB3	4:K:3043:HOH:O	1.60	1.01
2:K:230:CYS:SG	2:L:230:CYS:SG	2.59	1.01
1:C:76:CYS:CB	1:C:82:THR:HG22	1.91	1.00
2:D:192:PHE:CD1	2:D:194:GLU:HG2	1.97	1.00
1:C:76:CYS:HB2	1:C:82:THR:CG2	1.92	0.98
2:E:230:CYS:SG	2:F:230:CYS:SG	2.61	0.98
1:C:76:CYS:HB2	1:C:82:THR:HG22	1.00	0.97
2:J:129:THR:O	2:J:130:ARG:HB3	1.64	0.95
1:G:93:GLU:HG2	1:G:94:GLU:N	1.82	0.94
1:G:93:GLU:HG2	1:G:94:GLU:H	1.32	0.93
2:D:129:THR:O	2:D:130:ARG:HB3	1.68	0.93
1:H:118:THR:HG1	1:H:120:TRP:HE3	1.13	0.93
2:D:281:GLY:HA3	2:E:121:ARG:HG2	1.51	0.93
3:K:2:ZN:ZN	2:L:230:CYS:HG	0.62	0.91
1:C:92:ARG:HH11	1:C:92:ARG:HG3	1.34	0.91
2:J:230:CYS:SG	2:L:230:CYS:SG	2.69	0.90
2:J:281:GLY:HA3	2:K:121:ARG:HG2	1.54	0.90
2:J:121:ARG:HB3	2:L:281:GLY:HA2	1.52	0.90

![](_page_12_Picture_9.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	overlap (Å)
1:H:24:SER:O	1:H:25:GLU:HB2	1.72	0.89
1:G:99:MET:HE1	2:J:191:ARG:HH11	1.37	0.88
1:C:118:THR:HG1	1:C:120:TRP:HE3	1.20	0.88
1:I:117:CYS:O	1:I:118:THR:N	2.06	0.88
2:D:230:CYS:SG	2:F:230:CYS:SG	2.72	0.88
1:B:31:GLY:HA2	1:B:78:THR:O	1.74	0.87
3:E:1:ZN:ZN	2:F:230:CYS:HG	0.85	0.86
1:A:36:GLU:HG3	1:A:58:LEU:HD21	1.56	0.86
1:G:52:THR:HB	1:G:79:THR:O	1.77	0.85
1:C:89:GLY:HA2	4:C:3028:HOH:O	1.74	0.85
1:B:113:LYS:HG2	1:B:115:GLY:O	1.77	0.85
1:H:90:THR:HG22	1:H:102:LYS:HA	1.59	0.85
1:G:85:GLN:NE2	1:G:119:PRO:HG3	1.92	0.84
1:B:64:THR:H	1:B:81:ASN:HD21	1.23	0.84
1:G:36:GLU:HG3	1:G:58:LEU:HD21	1.59	0.84
1:G:112:VAL:HG13	1:G:126:VAL:HG12	1.58	0.83
2:D:149:ARG:HB2	4:D:3025:HOH:O	1.77	0.83
2:D:228:ASN:ND2	2:E:239:LEU:H	1.77	0.83
1:H:61:LEU:HD13	2:K:132:ARG:HH12	1.44	0.82
1:H:76:CYS:HB2	1:H:82:THR:HG22	1.62	0.82
2:L:129:THR:O	2:L:130:ARG:HB3	1.80	0.81
1:A:49:ASP:HB2	1:A:60:CYS:HB3	1.60	0.81
1:H:62:ARG:HG3	1:H:62:ARG:HH11	1.46	0.81
1:C:92:ARG:HG3	1:C:92:ARG:NH1	1.92	0.81
2:E:230:CYS:HG	3:E:1:ZN:ZN	0.92	0.81
1:A:80:ARG:NH1	1:A:80:ARG:HG2	1.96	0.80
1:C:62:ARG:HD2	2:F:131:GLY:HA2	1.63	0.80
2:D:228:ASN:HD22	2:E:239:LEU:H	1.29	0.80
1:G:86:CYS:SG	1:G:92:ARG:HD3	2.21	0.80
1:B:31:GLY:N	1:B:79:THR:HG22	1.97	0.80
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.46	0.80
2:L:132:ARG:HG3	2:L:270:HIS:CE1	2.16	0.79
2:L:132:ARG:HG3	2:L:270:HIS:HE1	1.47	0.79
1:G:115:GLY:HA3	1:G:124:GLU:HB2	1.64	0.79
2:D:199:ASN:C	4:D:3157:HOH:O	2.21	0.79
2:D:121:ARG:HB3	2:F:281:GLY:HA2	1.62	0.79
2:K:129:THR:HG22	2:K:155:GLU:HG2	1.63	0.79
1:B:76:CYS:HB2	1:B:82:THR:HG22	1.65	0.79
2:L:132:ARG:HH21	2:L:135:THR:HG21	1.48	0.79
1:H:64:THR:O	1:H:82:THR:HG21	1.84	0.78
2:L:181:PHE:HB2	2:L:280:VAL:CG2	2.13	0.78

![](_page_13_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:92:ARG:HG2	1:B:97:PRO:HA	1.66	0.77
1:C:46:TYR:CD1	2:L:168:HIS:HE1	2.02	0.77
2:F:181:PHE:HB2	2:F:280:VAL:CG2	2.15	0.77
2:D:132:ARG:HB2	2:D:270:HIS:CE1	2.20	0.77
1:A:44:CYS:SG	1:A:50:TYR:HA	2.26	0.76
2:L:132:ARG:HH21	2:L:135:THR:CG2	1.96	0.76
2:F:132:ARG:HH21	2:F:135:THR:HG21	1.48	0.76
2:J:132:ARG:HB2	2:J:270:HIS:CE1	2.21	0.76
1:C:28:CYS:SG	1:C:34:ILE:HD12	2.25	0.76
2:K:191:ARG:HG3	2:K:239:LEU:HD23	1.68	0.76
2:F:132:ARG:HH21	2:F:135:THR:CG2	1.98	0.76
1:I:48:GLN:O	1:I:63:CYS:SG	2.43	0.76
2:J:228:ASN:ND2	2:K:239:LEU:H	1.82	0.76
1:B:129:GLU:O	1:B:130:SER:OG	2.04	0.76
2:F:132:ARG:HG3	2:F:270:HIS:CE1	2.21	0.76
2:E:191:ARG:HG3	2:E:239:LEU:HD23	1.68	0.75
2:J:121:ARG:CB	2:L:281:GLY:HA2	2.16	0.75
1:G:93:GLU:OE1	1:G:95:ASP:HB2	1.87	0.75
2:E:129:THR:HG22	2:E:155:GLU:HG2	1.67	0.75
1:C:119:PRO:HD2	1:C:120:TRP:CZ3	2.21	0.75
1:A:49:ASP:HB2	1:A:60:CYS:CB	2.17	0.74
1:I:62:ARG:HB3	1:I:62:ARG:NH1	2.01	0.74
1:C:33:HIS:HD2	1:C:34:ILE:O	1.71	0.74
1:C:46:TYR:CE1	2:L:168:HIS:HE1	2.06	0.74
1:A:45:LYS:HE2	1:A:48:GLN:HE21	1.52	0.73
1:A:86:CYS:SG	1:A:92:ARG:HD3	2.27	0.73
2:D:132:ARG:HB2	2:D:270:HIS:HE1	1.54	0.73
1:G:91:PHE:CZ	1:G:122:ASP:HB2	2.24	0.72
1:B:112:VAL:HG22	1:B:126:VAL:HG23	1.72	0.72
2:J:231:TRP:CG	2:K:235:ALA:HA	2.25	0.72
2:K:132:ARG:HH21	2:K:135:THR:HG21	1.54	0.71
1:B:111:MET:HE2	1:B:125:CYS:HB2	1.71	0.71
1:G:99:MET:CE	2:J:191:ARG:HH11	2.02	0.71
2:J:228:ASN:HD22	2:K:239:LEU:H	1.37	0.71
1:C:62:ARG:O	2:F:132:ARG:HD3	1.91	0.70
1:G:99:MET:CE	2:J:191:ARG:HD2	2.21	0.70
1:I:49:ASP:HB2	1:I:60:CYS:HB2	1.72	0.70
1:B:113:LYS:HD3	1:B:116:ASP:OD1	1.90	0.70
2:D:126:ILE:HA	2:D:162:SER:HB2	1.73	0.70
1:H:62:ARG:HG3	1:H:62:ARG:NH1	2.03	0.70
1:H:42:ILE:H	1:H:42:ILE:HD12	1.56	0.70

![](_page_14_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:175:VAL:HG22	2:K:255:ARG:HG2	1.74	0.70
2:F:132:ARG:HG3	2:F:270:HIS:HE1	1.57	0.70
1:I:119:PRO:HD2	1:I:120:TRP:CZ3	2.27	0.70
1:B:27:LEU:HD22	1:B:55:ASN:O	1.91	0.69
2:J:126:ILE:HA	2:J:162:SER:HB2	1.74	0.69
1:I:118:THR:HG1	1:I:120:TRP:HE3	1.40	0.69
1:C:99:MET:HG3	2:F:239:LEU:HD21	1.74	0.69
1:G:31:GLY:HA2	1:G:78:THR:O	1.91	0.69
2:J:194:GLU:HG3	2:J:204:LYS:HE2	1.75	0.69
2:J:132:ARG:HB2	2:J:270:HIS:HE1	1.57	0.69
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.06	0.69
1:C:65:ARG:HD2	2:F:130:ARG:O	1.93	0.69
2:J:120:GLN:OE1	2:J:120:GLN:HA	1.92	0.69
2:D:121:ARG:CB	2:F:281:GLY:HA2	2.23	0.69
2:J:192:PHE:CD1	2:J:194:GLU:HB2	2.28	0.69
1:B:111:MET:HG3	2:D:199:ASN:ND2	2.09	0.68
1:B:61:LEU:HD13	2:E:132:ARG:HH12	1.57	0.68
1:C:49:ASP:O	1:C:50:TYR:HB3	1.92	0.68
1:C:78:THR:HG21	4:L:3018:HOH:O	1.94	0.68
1:B:59:PHE:HZ	2:E:158:ARG:HD2	1.59	0.68
1:A:80:ARG:CG	1:A:80:ARG:HH11	2.06	0.68
2:D:120:GLN:HA	2:D:120:GLN:OE1	1.93	0.68
1:G:73:LEU:HD21	1:G:85:GLN:OE1	1.94	0.67
1:C:46:TYR:CD1	2:L:168:HIS:CE1	2.83	0.67
2:F:129:THR:O	2:F:130:ARG:HB3	1.93	0.67
1:B:33:HIS:HD2	1:B:34:ILE:O	1.77	0.67
1:C:53:HIS:HB3	2:E:217:PRO:HG2	1.77	0.67
1:I:64:THR:O	1:I:82:THR:HG21	1.94	0.67
1:I:26:GLY:O	1:I:27:LEU:HD12	1.93	0.67
2:L:170:ARG:O	2:L:171:ASN:HB2	1.94	0.67
2:E:279:LEU:O	2:E:280:VAL:HG13	1.93	0.67
1:I:33:HIS:HD2	1:I:34:ILE:O	1.77	0.67
1:G:125:CYS:HB2	2:L:199:ASN:HD21	1.60	0.67
2:K:129:THR:CG2	2:K:155:GLU:HG2	2.24	0.67
2:D:185:TYR:OH	2:F:247:ILE:HG13	1.95	0.67
1:G:26:GLY:O	1:G:27:LEU:HD23	1.95	0.66
1:B:111:MET:CE	2:D:199:ASN:ND2	2.58	0.66
2:F:133:SER:OG	2:F:271:GLU:OE1	2.13	0.66
1:H:64:THR:H	1:H:81:ASN:HD21	1.42	0.66
2:J:192:PHE:HD1	2:J:194:GLU:HB2	1.61	0.66
2:F:170:ARG:O	2:F:171:ASN:HB2	1.96	0.66

![](_page_15_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
2:K:231:TRP:CH2	2:L:236:GLU:HB2	2.31	0.66
1:C:64:THR:HG21	2:F:134:ASN:HA	1.78	0.65
2:K:279:LEU:O	2:K:280:VAL:HG13	1.97	0.65
2:D:129:THB:HG23	2:D:155:GLU:HG2	1.78	0.65
2:D:192:PHE:HD1	2:D:194:GLU:HG2	1.57	0.65
2:F:166:ASN:O	2:F:167:LEU:HD12	1.97	0.65
1:B:108:PRO:HG3	2:D:199:ASN:O	1.96	0.65
2:E:175:VAL:HG22	2:E:255:ARG:HG2	1.79	0.65
1:B:44:CYS:HA	4:B:3144:HOH:O	1.96	0.65
2:D:129:THR:CG2	2:D:155:GLU:HG2	2.27	0.64
1:G:36:GLU:HA	1:G:58:LEU:HD11	1.77	0.64
1:B:111:MET:HB2	1:B:125:CYS:HB3	1.79	0.64
1:H:33:HIS:HB2	1:H:57:LEU:O	1.98	0.64
1:B:114:VAL:N	1:B:124:GLU:O	2.31	0.64
1:G:50:TYR:O	1:G:60:CYS:HB3	1.97	0.64
2:E:132:ARG:HH21	2:E:135:THR:HG21	1.63	0.64
2:K:247:ILE:HD11	2:L:278:PHE:HD2	1.63	0.64
2:E:231:TRP:CG	2:F:235:ALA:HA	2.33	0.63
1:A:45:LYS:HB3	1:A:48:GLN:HB2	1.80	0.63
1:I:42:ILE:HG22	1:I:43:SER:N	2.13	0.63
1:A:99:MET:HE2	2:D:191:ARG:HD2	1.79	0.63
1:B:111:MET:HA	1:B:126:VAL:O	1.99	0.63
1:B:64:THR:N	1:B:81:ASN:HD21	1.96	0.63
2:D:132:ARG:HH21	2:D:135:THR:HG21	1.64	0.63
2:E:231:TRP:CH2	2:F:236:GLU:HB2	2.34	0.62
2:J:121:ARG:HG2	2:L:281:GLY:CA	2.29	0.62
2:D:231:TRP:CG	2:E:235:ALA:HA	2.34	0.62
1:G:104:ARG:HD2	1:G:122:ASP:OD2	1.99	0.62
2:K:192:PHE:HD1	2:K:194:GLU:HB3	1.65	0.62
2:L:152:ASN:HA	2:L:172:GLY:HA3	1.82	0.62
1:A:45:LYS:HE2	1:A:48:GLN:NE2	2.14	0.62
2:E:181:PHE:O	2:E:279:LEU:HD12	2.00	0.62
2:K:168:HIS:HD1	2:K:177:HIS:HE2	1.46	0.62
2:D:174:LEU:HD12	2:D:275:PHE:CE2	2.35	0.62
2:E:190:PHE:CD1	2:E:206:MET:HG2	2.34	0.62
1:I:45:LYS:HD3	1:I:48:GLN:NE2	2.14	0.62
1:C:77:THR:HG21	1:C:80:ARG:NH1	2.14	0.62
1:I:26:GLY:C	1:I:27:LEU:HD12	2.20	0.62
1:I:31:GLY:N	1:I:79:THR:HG22	2.15	0.62
2:J:129:THR:HG23	2:J:155:GLU:HG2	1.82	0.61
2:L:166:ASN:O	2:L:167:LEU:HD12	2.00	0.61

![](_page_16_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:121:ARG:CG	2:L:281:GLY:HA2	2.30	0.61
1:A:99:MET:HE1	2:D:191:ARG:HG3	1.82	0.61
1:B:28:CYS:O	1:B:54:TRP:HA	2.00	0.61
2:J:129:THR:O	2:J:130:ARG:CB	2.42	0.61
1:I:53:HIS:CG	2:K:217:PRO:HG2	2.35	0.61
1:B:59:PHE:CZ	2:E:158:ARG:HD2	2.35	0.61
2:J:174:LEU:HD12	2:J:275:PHE:CE2	2.36	0.61
1:H:33:HIS:HD2	1:H:60:CYS:SG	2.24	0.61
2:E:247:ILE:HG13	2:F:185:TYR:OH	2.00	0.61
2:D:129:THR:O	2:D:130:ARG:CB	2.45	0.61
2:D:252:GLU:O	2:D:253:ASN:HB2	2.00	0.60
2:D:281:GLY:HA3	2:E:121:ARG:CG	2.27	0.60
1:I:62:ARG:HH11	1:I:62:ARG:HB3	1.64	0.60
1:C:50:TYR:HE2	1:C:61:LEU:HD12	1.66	0.60
2:J:192:PHE:HB3	2:J:265:LEU:HD22	1.82	0.60
1:I:61:LEU:HD13	2:L:132:ARG:NH1	2.15	0.60
1:A:90:THR:HB	1:A:100:CYS:HB3	1.83	0.60
2:L:233:LYS:HG3	2:L:234:ASP:OD1	2.01	0.60
2:J:121:ARG:HG2	2:L:281:GLY:HA2	1.82	0.60
1:A:44:CYS:SG	1:A:50:TYR:CA	2.89	0.60
2:E:129:THR:CG2	2:E:155:GLU:HG2	2.31	0.60
1:H:62:ARG:CG	1:H:62:ARG:HH11	2.15	0.60
1:B:59:PHE:CE2	2:E:159:SER:HA	2.36	0.60
2:F:164:LEU:HD22	2:F:168:HIS:HA	1.82	0.60
1:H:117:CYS:SG	1:H:118:THR:N	2.74	0.60
1:I:42:ILE:HD12	1:I:42:ILE:N	2.16	0.60
2:F:152:ASN:HA	2:F:172:GLY:HA3	1.84	0.60
1:B:111:MET:HE2	2:D:199:ASN:ND2	2.17	0.60
1:I:91:PHE:HD2	1:I:92:ARG:O	1.85	0.60
2:F:233:LYS:HG3	2:F:234:ASP:OD1	2.02	0.60
1:H:55:ASN:HB2	1:H:57:LEU:HG	1.84	0.60
2:L:149:ARG:HD3	2:L:263:GLU:CD	2.22	0.59
2:L:280:VAL:HG23	2:L:281:GLY:N	2.15	0.59
1:C:61:LEU:HD13	2:F:132:ARG:HH12	1.68	0.59
2:K:197:LYS:N	2:K:202:ASN:HD21	2.00	0.59
2:E:197:LYS:N	2:E:202:ASN:HD21	2.00	0.59
1:I:59:PHE:CZ	2:L:158:ARG:HD2	2.37	0.59
1:A:58:LEU:HD22	2:D:158:ARG:NH1	2.18	0.59
1:B:58:LEU:O	4:B:3141:HOH:O	2.17	0.59
1:I:61:LEU:HD13	2:L:132:ARG:HH12	1.67	0.59
2:L:200:THR:HG22	2:L:201:LYS:N	2.18	0.59

![](_page_17_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:50:TYR:CZ	1:B:81:ASN:HB2	2.38	0.59
1:G:50:TYR:CZ	1:G:81:ASN:HB2	2.38	0.59
1:A:48:GLN:O	1:A:63:CYS:SG	2.61	0.59
1:A:118:THR:HB	1:A:119:PRO:HD2	1.83	0.58
2:D:263:GLU:HB3	4:D:3025:HOH:O	2.03	0.58
2:E:189:TYR:OH	2:E:239:LEU:HD22	2.03	0.58
2:K:181:PHE:O	2:K:279:LEU:HD12	2.03	0.58
2:J:130:ARG:O	2:J:130:ARG:HG3	2.03	0.58
2:J:129:THR:CG2	2:J:155:GLU:HG2	2.32	0.58
2:L:149:ARG:NH1	4:L:3074:HOH:O	2.35	0.58
2:L:252:GLU:O	2:L:253:ASN:HB2	2.03	0.58
2:L:164:LEU:HD22	2:L:168:HIS:HA	1.85	0.58
2:K:173:GLU:HG2	2:K:257:PHE:HB3	1.86	0.58
1:A:42:ILE:N	1:A:42:ILE:HD12	2.18	0.58
2:D:130:ARG:HG3	2:D:130:ARG:O	2.03	0.58
1:G:99:MET:HG2	2:J:237:TYR:CD1	2.38	0.58
1:B:56:ASP:N	1:B:56:ASP:OD1	2.37	0.58
2:D:121:ARG:CG	2:F:281:GLY:HA2	2.33	0.58
1:I:33:HIS:HB2	1:I:57:LEU:O	2.04	0.58
1:B:81:ASN:ND2	1:B:82:THR:H	2.02	0.57
2:F:149:ARG:HD3	2:F:263:GLU:CD	2.25	0.57
2:J:281:GLY:HA3	2:K:121:ARG:CG	2.30	0.57
1:G:93:GLU:CD	1:G:95:ASP:HB2	2.24	0.57
1:H:52:THR:HB	1:H:79:THR:O	2.03	0.57
2:D:121:ARG:HG2	2:F:281:GLY:HA2	1.85	0.57
1:C:50:TYR:CE2	1:C:61:LEU:HD12	2.40	0.57
2:E:173:GLU:HG2	2:E:257:PHE:HB3	1.86	0.57
1:B:90:THR:HB	1:B:100:CYS:HB3	1.85	0.57
1:C:92:ARG:HD3	1:C:97:PRO:HA	1.86	0.57
1:I:52:THR:HB	1:I:79:THR:O	2.04	0.57
2:K:231:TRP:CG	2:L:235:ALA:HA	2.39	0.57
1:A:64:THR:HA	2:D:132:ARG:O	2.04	0.57
1:C:87:GLU:CD	1:C:88:GLU:H	2.07	0.57
2:D:194:GLU:HG3	4:D:3088:HOH:O	2.05	0.57
1:H:23:PRO:HD3	1:H:41:CYS:SG	2.45	0.57
1:C:73:LEU:HB3	1:C:83:VAL:HG12	1.85	0.57
1:C:33:HIS:CD2	1:C:34:ILE:O	2.57	0.57
2:L:200:THR:HG22	2:L:201:LYS:H	1.70	0.57
1:G:52:THR:OG1	1:G:52:THR:O	2.23	0.56
2:K:161:HIS:CD2	2:K:161:HIS:N	2.73	0.56
1:C:44:CYS:SG	1:C:50:TYR:HA	2.45	0.56

![](_page_18_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	overlap (Å)
2:E:161:HIS:CD2	2:E:161:HIS:N	2.73	0.56
2:E:187:GLN:NE2	2:E:274:PHE:CZ	2.73	0.56
2:F:126:ILE:HD12	2:F:154:TRP:CB	2.34	0.56
2:F:209:TYR:HD1	2:F:221:LEU:HD11	1.70	0.56
2:D:121:ARG:HG2	2:F:281:GLY:CA	2.35	0.56
2:L:125:HIS:HE1	2:L:274:PHE:CD1	2.23	0.56
2:K:192:PHE:CD1	2:K:194:GLU:HB3	2.39	0.56
2:E:127:THR:HG22	2:E:274:PHE:HB3	1.85	0.56
2:E:264:HIS:O	2:E:265:LEU:HD23	2.05	0.56
1:B:24:SER:O	1:B:25:GLU:HB2	2.05	0.56
2:F:147:LEU:HB2	2:F:211:TYR:OH	2.05	0.56
1:H:31:GLY:HA2	1:H:78:THR:O	2.04	0.56
1:C:55:ASN:HB2	1:C:57:LEU:HG	1.88	0.56
1:C:78:THR:HG23	1:C:79:THR:HG23	1.88	0.56
1:C:57:LEU:HD21	2:E:216:TYR:CD1	2.41	0.56
2:L:280:VAL:HG23	2:L:281:GLY:H	1.70	0.56
1:C:67:ASP:O	1:C:70:GLU:HB2	2.05	0.56
1:B:91:PHE:CE1	1:B:122:ASP:HB2	2.41	0.55
1:C:53:HIS:CB	2:E:217:PRO:HG2	2.36	0.55
1:C:34:ILE:HG23	1:C:35:SER:N	2.22	0.55
1:H:67:ASP:CG	2:K:191:ARG:HH22	2.09	0.55
2:F:252:GLU:O	2:F:253:ASN:HB2	2.07	0.55
2:F:280:VAL:HG23	2:F:281:GLY:N	2.20	0.55
1:C:118:THR:OG1	1:C:120:TRP:HE3	1.86	0.55
1:C:122:ASP:OD2	2:E:201:LYS:HD2	2.07	0.55
2:J:226:ALA:H	2:K:241:SER:HB2	1.72	0.55
1:H:22:SER:HB3	1:H:23:PRO:HD2	1.88	0.55
2:L:127:THR:OG1	2:L:270:HIS:HB2	2.07	0.55
1:B:112:VAL:O	1:B:125:CYS:HA	2.07	0.55
1:I:93:GLU:HB3	1:I:96:SER:OG	2.07	0.55
2:L:133:SER:OG	2:L:271:GLU:OE1	2.25	0.55
2:F:126:ILE:HA	2:F:162:SER:HB2	1.89	0.54
1:G:23:PRO:HB3	1:G:34:ILE:HD12	1.88	0.54
1:A:26:GLY:O	1:A:27:LEU:HD23	2.07	0.54
4:E:3118:HOH:O	2:F:270:HIS:HD2	1.90	0.54
1:I:28:CYS:O	1:I:54:TRP:HA	2.08	0.54
2:D:174:LEU:HD12	2:D:275:PHE:CZ	2.43	0.54
2:J:132:ARG:HH21	2:J:135:THR:HG21	1.73	0.54
2:K:247:ILE:HG13	2:L:185:TYR:OH	2.07	0.54
1:H:52:THR:OG1	1:H:52:THR:O	2.24	0.54
1:C:99:MET:HG3	2:F:239:LEU:CD2	2.38	0.54

![](_page_19_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:50:TYR:CD2	1:C:50:TYR:C	2.82	0.54
1:C:87:GLU:HG3	1:C:88:GLU:N	2.23	0.54
2:K:156:SER:HB3	2:K:169:LEU:HD23	1.89	0.53
2:E:189:TYR:HD2	2:E:272:ALA:HB1	1.73	0.53
1:C:87:GLU:CG	1:C:88:GLU:N	2.72	0.53
1:H:23:PRO:HG2	1:H:38:GLY:O	2.09	0.53
1:A:101:ARG:HH21	2:F:201:LYS:HE2	1.73	0.53
2:E:192:PHE:HD1	2:E:194:GLU:HB3	1.73	0.53
2:D:236:GLU:HB2	2:F:231:TRP:CH2	2.44	0.53
1:B:96:SER:N	1:B:97:PRO:HD3	2.24	0.53
1:H:64:THR:N	1:H:81:ASN:HD21	2.06	0.53
2:K:189:TYR:HD2	2:K:272:ALA:HB1	1.74	0.53
1:I:59:PHE:HZ	2:L:158:ARG:HD2	1.73	0.53
1:B:111:MET:CA	1:B:126:VAL:O	2.57	0.53
1:G:108:PRO:O	1:G:111:MET:HB2	2.09	0.53
2:J:184:ILE:HD11	2:J:250:LEU:HD11	1.91	0.53
1:C:32:HIS:ND1	1:C:43:SER:HB3	2.24	0.53
1:C:44:CYS:HB3	1:C:49:ASP:OD1	2.09	0.53
1:C:33:HIS:HB2	1:C:57:LEU:O	2.09	0.53
2:F:156:SER:HB3	2:F:169:LEU:HD23	1.90	0.53
1:H:63:CYS:HA	1:H:81:ASN:ND2	2.24	0.53
1:I:42:ILE:N	1:I:42:ILE:CD1	2.72	0.53
2:D:127:THR:OG1	2:D:270:HIS:HB2	2.09	0.52
2:J:184:ILE:O	2:J:245:GLY:HA2	2.09	0.52
2:L:126:ILE:HA	2:L:162:SER:HB2	1.90	0.52
1:C:62:ARG:CD	2:F:131:GLY:HA2	2.34	0.52
1:G:122:ASP:OD1	1:G:123:ILE:N	2.42	0.52
2:J:127:THR:OG1	2:J:270:HIS:HB2	2.08	0.52
2:L:126:ILE:CD1	2:L:169:LEU:HD13	2.40	0.52
1:A:85:GLN:NE2	1:A:119:PRO:HG3	2.24	0.52
1:B:129:GLU:C	1:B:130:SER:OG	2.48	0.52
1:B:52:THR:O	1:B:52:THR:OG1	2.26	0.52
1:H:61:LEU:HD13	2:K:132:ARG:NH1	2.20	0.52
1:B:108:PRO:HD2	1:B:111:MET:HG3	1.91	0.52
1:H:99:MET:CE	2:K:191:ARG:HE	2.22	0.52
1:I:34:ILE:HG13	1:I:35:SER:H	1.75	0.52
2:L:209:TYR:HD1	2:L:221:LEU:HD11	1.75	0.52
1:B:128:LYS:HG3	1:B:128:LYS:O	2.10	0.52
2:F:126:ILE:HD12	2:F:154:TRP:HB3	1.91	0.52
1:A:50:TYR:CZ	1:A:81:ASN:HB2	2.44	0.52
1:H:28:CYS:O	1:H:54:TRP:HA	2.10	0.52

![](_page_20_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:73:LEU:HD21	1:H:85:GLN:OE1	2.09	0.52
1:I:30:PRO:O	1:I:32:HIS:HD2	1.93	0.52
2:L:147:LEU:HB2	2:L:211:TYR:OH	2.10	0.52
2:L:208:GLN:NE2	2:L:210:ILE:HD11	2.25	0.52
1:B:91:PHE:CZ	1:B:122:ASP:HB2	2.45	0.52
2:D:121:ARG:CZ	2:F:181:PHE:CE2	2.93	0.52
2:E:168:HIS:HD1	2:E:177:HIS:HE2	1.58	0.52
2:F:132:ARG:NH2	2:F:135:THR:HG21	2.22	0.52
1:I:59:PHE:HZ	2:L:158:ARG:HH11	1.55	0.52
2:L:270:HIS:CD2	2:L:271:GLU:HG3	2.45	0.52
1:C:77:THR:OG1	1:C:80:ARG:HB3	2.10	0.51
1:G:92:ARG:HG2	1:G:97:PRO:HA	1.92	0.51
1:I:70:GLU:HA	1:I:85:GLN:O	2.10	0.51
1:I:99:MET:HG3	2:L:239:LEU:HD21	1.91	0.51
2:J:247:ILE:HD12	2:K:185:TYR:OH	2.10	0.51
1:B:112:VAL:CG2	1:B:126:VAL:HG23	2.40	0.51
1:C:96:SER:N	1:C:97:PRO:HD3	2.26	0.51
1:B:61:LEU:HD13	2:E:132:ARG:NH1	2.24	0.51
2:E:247:ILE:HD11	2:F:278:PHE:HD2	1.76	0.51
2:E:187:GLN:NE2	2:E:274:PHE:HZ	2.09	0.51
1:H:49:ASP:OD1	1:H:60:CYS:HB2	2.11	0.51
2:J:190:PHE:CZ	2:J:266:ILE:HD11	2.46	0.51
1:B:114:VAL:HB	1:B:126:VAL:HG22	1.92	0.51
2:D:190:PHE:CZ	2:D:266:ILE:HD11	2.45	0.51
2:F:270:HIS:CD2	2:F:271:GLU:HG3	2.46	0.51
2:J:236:GLU:HB2	2:L:231:TRP:CH2	2.45	0.51
2:K:187:GLN:NE2	2:K:274:PHE:CZ	2.79	0.51
1:H:99:MET:HE1	2:K:191:ARG:HG2	1.91	0.51
2:L:192:PHE:HE1	2:L:194:GLU:OE2	1.94	0.51
2:F:125:HIS:HE1	2:F:274:PHE:CD1	2.30	0.50
2:E:252:GLU:HG2	2:E:253:ASN:OD1	2.11	0.50
1:G:70:GLU:OE2	2:J:134:ASN:ND2	2.44	0.50
2:F:187:GLN:HA	2:F:242:ILE:O	2.12	0.50
2:F:127:THR:OG1	2:F:270:HIS:HB2	2.10	0.50
2:F:181:PHE:HB2	2:F:280:VAL:HG21	1.91	0.50
1:I:64:THR:HG22	1:I:65:ARG:N	2.26	0.50
1:A:122:ASP:OD1	1:A:123:ILE:HG13	2.11	0.50
2:E:199:ASN:O	2:E:200:THR:HG23	2.11	0.50
1:G:37:ASP:C	1:G:37:ASP:OD1	2.50	0.50
1:G:45:LYS:HD3	1:G:48:GLN:CD	2.31	0.50
1:H:53:HIS:CG	2:J:217:PRO:HG2	2.47	0.50

![](_page_21_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:D:189:TYR:OH	2:D:239:LEU:HD22	2.11	0.50
2:E:251:LYS:O	2:E:254:ASP:HB2	2.12	0.50
1:G:97:PRO:HG2	2:L:209:TYR:OH	2.12	0.50
2:E:218:ASP:HB3	2:E:219:PRO:HD2	1.93	0.50
2:F:278:PHE:HD1	2:F:279:LEU:O	1.95	0.50
2:E:192:PHE:CD1	2:E:194:GLU:HB3	2.47	0.50
1:H:119:PRO:HD2	1:H:120:TRP:CZ3	2.47	0.50
2:F:155:GLU:OE1	2:F:161:HIS:HE1	1.94	0.50
2:D:194:GLU:CB	4:D:3088:HOH:O	2.59	0.50
2:E:189:TYR:HH	2:E:239:LEU:HD22	1.77	0.50
2:L:132:ARG:NH2	2:L:135:THR:HG21	2.21	0.50
2:J:185:TYR:OH	2:L:247:ILE:HG13	2.11	0.50
1:C:59:PHE:HZ	2:F:158:ARG:HH11	1.59	0.49
1:I:31:GLY:C	1:I:32:HIS:CD2	2.85	0.49
2:K:127:THR:HG22	2:K:274:PHE:HB3	1.93	0.49
1:B:122:ASP:OD1	1:B:123:ILE:N	2.45	0.49
2:E:194:GLU:O	2:E:194:GLU:HG3	2.09	0.49
2:L:184:ILE:O	2:L:245:GLY:HA2	2.11	0.49
1:A:56:ASP:N	1:A:56:ASP:OD1	2.45	0.49
1:B:113:LYS:CD	1:B:116:ASP:OD1	2.60	0.49
2:F:209:TYR:HB3	2:F:221:LEU:CD1	2.42	0.49
1:A:44:CYS:SG	1:A:50:TYR:C	2.91	0.49
2:E:190:PHE:CE1	2:E:266:ILE:HD11	2.48	0.49
1:H:92:ARG:HG2	1:H:97:PRO:HA	1.95	0.49
1:I:92:ARG:HG2	1:I:93:GLU:H	1.77	0.49
1:C:23:PRO:HD3	1:C:39:ARG:O	2.13	0.49
2:E:182:TYR:O	2:E:247:ILE:HA	2.13	0.49
1:G:49:ASP:O	1:G:50:TYR:HB3	2.13	0.49
1:I:67:ASP:O	1:I:70:GLU:HB2	2.12	0.49
1:A:30:PRO:O	1:A:32:HIS:HD2	1.95	0.49
1:B:50:TYR:OH	1:B:81:ASN:HB2	2.12	0.49
1:C:32:HIS:CE1	1:C:43:SER:HB3	2.46	0.49
2:F:260:VAL:HG21	2:F:266:ILE:HD11	1.95	0.49
1:G:64:THR:HA	2:J:132:ARG:O	2.13	0.49
2:K:251:LYS:O	2:K:254:ASP:HB2	2.13	0.49
2:L:155:GLU:OE1	2:L:161:HIS:HE1	1.95	0.49
2:D:184:ILE:O	2:D:245:GLY:HA2	2.12	0.49
1:I:70:GLU:OE2	2:L:134:ASN:ND2	2.45	0.49
1:I:92:ARG:O	1:I:93:GLU:HB2	2.13	0.49
2:J:121:ARG:CG	2:L:281:GLY:CA	2.90	0.49
1:G:99:MET:HG2	2:J:237:TYR:CG	2.48	0.49

![](_page_22_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:133:SER:OG	2:D:271:GLU:OE1	2.21	0.49
2:L:204:LYS:HB2	2:L:229:SER:HB3	1.93	0.49
2:L:218:ASP:HB3	2:L:219:PRO:HD2	1.94	0.49
1:B:33:HIS:CD2	1:B:34:ILE:O	2.63	0.48
2:K:199:ASN:O	2:K:200:THR:HG23	2.13	0.48
2:L:209:TYR:HB3	2:L:221:LEU:CD1	2.42	0.48
1:H:119:PRO:HG2	1:H:120:TRP:CE2	2.48	0.48
1:A:118:THR:HB	1:A:119:PRO:CD	2.43	0.48
2:D:231:TRP:CH2	2:E:236:GLU:HB2	2.48	0.48
1:H:22:SER:HA	1:H:41:CYS:SG	2.54	0.48
1:A:65:ARG:HD3	1:A:66:CYS:O	2.13	0.48
1:C:32:HIS:HA	1:C:42:ILE:O	2.13	0.48
2:E:187:GLN:HA	2:E:242:ILE:O	2.14	0.48
1:I:29:PRO:O	1:I:30:PRO:C	2.50	0.48
2:K:190:PHE:CE1	2:K:266:ILE:HD11	2.48	0.48
1:C:52:THR:HG22	1:C:79:THR:C	2.34	0.48
2:K:182:TYR:CZ	2:K:279:LEU:HD13	2.49	0.48
1:C:32:HIS:HA	1:C:43:SER:HA	1.95	0.48
1:C:89:GLY:CA	4:C:3028:HOH:O	2.48	0.48
2:D:226:ALA:H	2:E:241:SER:HB2	1.79	0.48
2:F:126:ILE:CD1	2:F:169:LEU:HD13	2.44	0.48
2:F:280:VAL:HG23	2:F:281:GLY:H	1.77	0.48
1:I:42:ILE:CG2	1:I:43:SER:N	2.77	0.48
1:I:62:ARG:O	2:L:132:ARG:HD3	2.14	0.48
2:L:126:ILE:HD13	2:L:169:LEU:HD13	1.95	0.48
1:C:91:PHE:HE1	1:C:102:LYS:O	1.97	0.48
1:I:53:HIS:CB	2:K:217:PRO:HG2	2.44	0.48
2:J:199:ASN:C	2:J:200:THR:HG22	2.33	0.48
2:L:179:LYS:O	2:L:179:LYS:HG3	2.12	0.48
1:B:92:ARG:CG	1:B:97:PRO:HA	2.41	0.48
2:L:181:PHE:HB2	2:L:280:VAL:HG21	1.94	0.48
2:D:184:ILE:HD11	2:D:250:LEU:HD11	1.96	0.48
2:F:243:TYR:C	2:F:243:TYR:CD1	2.87	0.48
2:J:182:TYR:CZ	2:J:279:LEU:HD13	2.49	0.48
2:E:130:ARG:HH11	2:E:130:ARG:HG2	1.79	0.47
2:F:179:LYS:HG3	2:F:179:LYS:O	2.14	0.47
1:H:90:THR:HB	1:H:100:CYS:HB3	1.96	0.47
1:I:118:THR:C	1:I:120:TRP:H	2.18	0.47
2:J:174:LEU:HD12	2:J:275:PHE:CZ	2.48	0.47
1:G:73:LEU:HD22	1:G:85:GLN:HB2	1.96	0.47
2:K:228:ASN:ND2	2:L:239:LEU:H	2.12	0.47

![](_page_23_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:150:LYS:HA	2:E:259:SER:HA	1.97	0.47
2:J:207:VAL:HG13	2:J:226:ALA:HB2	1.95	0.47
2:J:231:TRP:CD2	2:K:235:ALA:HA	2.49	0.47
2:E:228:ASN:ND2	2:F:239:LEU:H	2.12	0.47
2:F:184:ILE:O	2:F:245:GLY:HA2	2.14	0.47
1:I:98:GLU:HG2	2:K:207:VAL:HG21	1.97	0.47
1:H:84:CYS:HB2	2:K:134:ASN:HD21	1.80	0.47
2:L:278:PHE:HD1	2:L:279:LEU:O	1.98	0.47
2:E:184:ILE:O	2:E:245:GLY:HA2	2.14	0.47
1:H:86:CYS:HB3	1:H:90:THR:O	2.15	0.47
1:I:46:TYR:CD1	1:I:47:GLY:N	2.82	0.47
2:J:121:ARG:HG2	2:L:281:GLY:HA3	1.96	0.47
1:B:108:PRO:HG3	2:D:199:ASN:C	2.29	0.47
1:C:50:TYR:HE1	1:C:81:ASN:OD1	1.98	0.47
2:J:197:LYS:HB3	2:J:200:THR:CG2	2.45	0.47
1:C:57:LEU:HB2	1:C:59:PHE:O	2.15	0.47
2:D:225:SER:OG	2:D:227:ARG:NH1	2.48	0.47
2:E:156:SER:HB3	2:E:169:LEU:HD23	1.97	0.47
1:G:45:LYS:HB2	1:G:48:GLN:HB2	1.96	0.47
1:H:67:ASP:OD2	2:K:191:ARG:NH2	2.39	0.47
2:J:190:PHE:CD2	2:J:206:MET:HG2	2.50	0.47
1:C:31:GLY:HA2	1:C:78:THR:O	2.15	0.47
1:C:76:CYS:H	2:L:170:ARG:NH1	2.13	0.47
2:J:222:LEU:C	2:J:223:MET:HG3	2.36	0.46
1:C:30:PRO:HD3	1:C:54:TRP:NE1	2.30	0.46
2:F:169:LEU:HG	2:F:170:ARG:N	2.30	0.46
2:K:194:GLU:HG3	2:K:194:GLU:O	2.11	0.46
2:F:208:GLN:NE2	2:F:210:ILE:HD11	2.30	0.46
2:F:238:GLY:C	2:F:239:LEU:HD23	2.35	0.46
1:G:112:VAL:HB	1:G:128:LYS:HD2	1.96	0.46
1:B:29:PRO:HA	1:B:54:TRP:CD2	2.51	0.46
2:F:126:ILE:HD13	2:F:169:LEU:HD13	1.98	0.46
1:G:36:GLU:C	1:G:38:GLY:N	2.69	0.46
1:H:50:TYR:CD2	1:H:50:TYR:C	2.88	0.46
1:C:61:LEU:HD13	2:F:132:ARG:NH1	2.31	0.46
1:C:87:GLU:CG	1:C:88:GLU:H	2.28	0.46
1:C:99:MET:HE1	2:F:193:GLN:HG3	1.96	0.46
1:G:67:ASP:C	1:G:67:ASP:OD1	2.54	0.46
2:E:182:TYR:CZ	2:E:279:LEU:HD13	2.50	0.46
2:F:280:VAL:CG2	2:F:281:GLY:H	2.29	0.46
1:I:31:GLY:CA	1:I:79:THR:HG22	2.45	0.46

![](_page_24_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:L:133:SER:O	2:L:134:ASN:C	2.54	0.46
1:A:49:ASP:HB2	1:A:60:CYS:HB2	1.95	0.46
1:A:46:TYR:CE2	1:A:77:THR:HA	2.51	0.46
1:B:52:THR:O	1:B:53:HIS:CG	2.69	0.46
1:C:96:SER:HB2	2:E:205:GLN:CD	2.36	0.46
1:G:50:TYR:OH	1:G:81:ASN:HB2	2.16	0.46
1:H:24:SER:HB2	1:H:54:TRP:HZ3	1.81	0.46
1:H:45:LYS:HG2	1:H:48:GLN:CB	2.46	0.46
2:L:156:SER:HB3	2:L:169:LEU:HD23	1.97	0.46
2:D:222:LEU:C	2:D:223:MET:HG3	2.35	0.46
1:A:97:PRO:HG2	2:F:209:TYR:OH	2.16	0.46
1:I:33:HIS:CD2	1:I:34:ILE:O	2.65	0.46
1:C:49:ASP:O	1:C:50:TYR:CB	2.63	0.46
2:D:127:THR:HG23	2:D:162:SER:HB3	1.98	0.46
2:E:207:VAL:HG13	2:E:226:ALA:HB2	1.96	0.46
2:E:189:TYR:CD2	2:E:272:ALA:HB1	2.51	0.46
2:F:209:TYR:CD1	2:F:221:LEU:HD11	2.50	0.46
1:G:96:SER:N	1:G:97:PRO:HD3	2.31	0.46
2:J:127:THR:HG23	2:J:162:SER:HB3	1.98	0.46
2:D:207:VAL:HG13	2:D:226:ALA:HB2	1.98	0.45
2:F:189:TYR:HD2	2:F:272:ALA:HB1	1.81	0.45
2:F:214:THR:O	2:F:216:TYR:N	2.48	0.45
1:I:85:GLN:NE2	1:I:119:PRO:HG2	2.31	0.45
2:J:187:GLN:HA	2:J:242:ILE:O	2.16	0.45
1:H:99:MET:HE1	2:K:191:ARG:HE	1.80	0.45
1:G:118:THR:C	1:G:120:TRP:H	2.19	0.45
2:L:243:TYR:CD1	2:L:243:TYR:C	2.89	0.45
1:B:27:LEU:HD22	1:B:55:ASN:C	2.37	0.45
2:D:175:VAL:HG22	2:D:255:ARG:HG2	1.97	0.45
2:D:214:THR:O	2:D:216:TYR:N	2.48	0.45
2:K:130:ARG:HH11	2:K:130:ARG:HG2	1.80	0.45
1:A:58:LEU:HD22	2:D:158:ARG:HH12	1.80	0.45
1:C:67:ASP:O	1:C:68:SER:C	2.54	0.45
2:F:149:ARG:NH1	4:F:3017:HOH:O	2.48	0.45
1:G:44:CYS:HB3	1:G:49:ASP:OD1	2.16	0.45
1:B:29:PRO:O	1:B:30:PRO:O	2.34	0.45
1:C:21:SER:HA	1:C:41:CYS:H	1.81	0.45
1:C:37:ASP:OD2	1:C:39:ARG:HB2	2.17	0.45
2:D:235:ALA:HA	2:F:231:TRP:CG	2.52	0.45
1:A:28:CYS:O	1:A:54:TRP:HA	2.17	$0.\overline{45}$
1:B:104:ARG:HB2	1:B:104:ARG:HE	1.71	0.45

![](_page_25_Picture_6.jpeg)

		Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:B:112:VAL:O	1:B:114:VAL:N	2.50	0.45		
1:I:52:THR:HG21	4:I:3040:HOH:O	2.16	0.45		
2:J:189:TYR:OH	2:J:239:LEU:HD22	2.16	0.45		
1:B:111:MET:CB	1:B:125:CYS:HB3	2.45	0.45		
1:C:74:SER:HA	1:C:75:PRO:HD2	1.74	0.45		
2:F:218:ASP:HB3	2:F:219:PRO:HD2	1.97	0.45		
2:D:121:ARG:CG	2:F:281:GLY:CA	2.95	0.45		
1:I:50:TYR:CE2	1:I:61:LEU:HD12	2.52	0.45		
2:K:152:ASN:HA	2:K:172:GLY:HA3	1.99	0.45		
2:L:208:GLN:O	2:L:224:LYS:HA	2.16	0.45		
1:B:112:VAL:N	1:B:126:VAL:O	2.49	0.45		
2:D:164:LEU:HD22	2:D:168:HIS:HA	1.97	0.45		
2:J:254:ASP:O	2:J:255:ARG:HG3	2.17	0.45		
2:K:189:TYR:OH	2:K:239:LEU:HD22	2.17	0.45		
1:C:98:GLU:OE2	2:E:224:LYS:NZ	2.47	0.45		
2:F:169:LEU:HD11	2:F:172:GLY:HA2	1.99	0.45		
2:K:168:HIS:ND1	2:K:177:HIS:NE2	2.58	0.45		
1:C:61:LEU:HB3	2:F:132:ARG:NH1	2.32	0.44		
2:E:161:HIS:ND1	2:E:270:HIS:CD2	2.85	0.44		
2:F:127:THR:HG23	2:F:162:SER:HB3	1.98	0.44		
2:J:252:GLU:O	2:J:253:ASN:HB2	2.16	0.44		
1:C:91:PHE:HD2	1:C:92:ARG:O	1.99	0.44		
1:C:92:ARG:O	1:C:93:GLU:HB2	2.17	0.44		
2:D:263:GLU:HA	2:D:266:ILE:HG12	1.99	0.44		
2:K:218:ASP:HB3	2:K:219:PRO:HD2	2.00	0.44		
2:L:189:TYR:CD2	2:L:272:ALA:HB1	2.51	0.44		
2:E:152:ASN:HA	2:E:172:GLY:HA3	1.99	0.44		
2:K:187:GLN:HA	2:K:242:ILE:O	2.17	0.44		
1:C:77:THR:C	1:C:79:THR:H	2.21	0.44		
2:E:231:TRP:CD2	2:F:235:ALA:HA	2.53	0.44		
1:H:91:PHE:HE1	1:H:102:LYS:O	2.00	0.44		
1:G:104:ARG:CD	1:G:122:ASP:OD2	2.66	0.44		
1:G:24:SER:O	1:G:25:GLU:HB2	2.17	0.44		
1:H:53:HIS:CB	2:J:217:PRO:HG2	2.48	0.44		
2:E:161:HIS:ND1	2:E:270:HIS:CG	2.85	0.44		
2:K:190:PHE:CD1	2:K:206:MET:HG2	2.53	0.44		
1:C:50:TYR:CE1	1:C:81:ASN:HA	2.53	0.44		
1:G:107:CYS:HB3	1:G:108:PRO:HD2	1.99	0.44		
1:I:98:GLU:O	1:I:99:MET:HG2	2.17	0.44		
1:B:45:LYS:HB2	1:B:48:GLN:HB3	1.99	0.44		
2:D:254:ASP:O	2:D:255:ARG:HG3	2.18	0.44		

![](_page_26_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:211:TYR:HB2	2:D:257:PHE:CZ	2.52	0.44
2:K:247:ILE:HD11	2:L:278:PHE:CD2	2.49	0.44
2:J:121:ARG:CZ	2:L:181:PHE:CE2	3.01	0.44
2:L:208:GLN:NE2	2:L:244:GLN:HE21	2.16	0.44
2:L:131:GLY:O	2:L:269:ASP:HA	2.18	0.44
1:A:62:ARG:HH22	2:D:129:THR:HG22	1.83	0.44
2:E:197:LYS:H	2:E:202:ASN:HD21	1.66	0.44
2:L:212:LYS:HG2	2:L:222:LEU:HD21	1.99	0.44
1:B:22:SER:HA	1:B:23:PRO:HD3	1.88	0.43
1:C:66:CYS:HB3	1:C:70:GLU:HB3	2.00	0.43
2:E:265:LEU:HA	4:E:3016:HOH:O	2.18	0.43
1:G:125:CYS:HB2	2:L:199:ASN:ND2	2.31	0.43
1:G:49:ASP:HB2	1:G:60:CYS:HB2	2.00	0.43
1:H:99:MET:HG3	1:H:100:CYS:N	2.33	0.43
1:A:24:SER:OG	1:A:54:TRP:CZ3	2.71	0.43
1:A:62:ARG:NH2	2:D:155:GLU:OE1	2.50	0.43
2:F:254:ASP:C	2:F:255:ARG:HG3	2.39	0.43
1:I:118:THR:O	1:I:120:TRP:N	2.51	0.43
1:C:77:THR:HG21	1:C:80:ARG:HH12	1.81	0.43
1:C:93:GLU:HG2	1:C:94:GLU:H	1.83	0.43
1:G:73:LEU:CD2	1:G:85:GLN:HB2	2.48	0.43
2:L:187:GLN:HA	2:L:242:ILE:O	2.17	0.43
1:A:119:PRO:HD2	1:A:120:TRP:CZ3	2.53	0.43
1:B:29:PRO:HB3	1:B:54:TRP:CH2	2.53	0.43
2:F:133:SER:O	2:F:134:ASN:C	2.57	0.43
1:H:56:ASP:OD1	1:H:56:ASP:N	2.52	0.43
2:J:183:TYR:O	2:J:277:ALA:HA	2.17	0.43
1:C:30:PRO:HD3	1:C:54:TRP:CD1	2.53	0.43
1:A:70:GLU:OE2	2:D:134:ASN:ND2	2.51	0.43
2:F:181:PHE:CD1	2:F:249:GLU:HG3	2.54	0.43
2:F:189:TYR:CD2	2:F:272:ALA:HB1	2.53	0.43
1:I:122:ASP:OD1	1:I:123:ILE:HG13	2.19	0.43
1:C:64:THR:HG22	1:C:65:ARG:N	2.34	0.43
2:E:279:LEU:HD12	2:E:279:LEU:HA	1.78	0.43
1:G:36:GLU:C	1:G:38:GLY:H	2.22	0.43
1:I:69:GLY:O	1:I:87:GLU:N	2.50	0.43
1:B:111:MET:HE2	1:B:125:CYS:CB	2.46	0.43
1:B:64:THR:O	1:B:82:THR:CG2	2.66	0.43
1:C:91:PHE:CE1	1:C:102:LYS:O	2.72	0.43
2:J:227:ARG:HA	2:K:239:LEU:O	2.18	0.43
2:K:182:TYR:O	2:K:247:ILE:HA	2.19	0.43

![](_page_27_Picture_6.jpeg)

		Interatomic	Clash	
Atom-1	Atom-2	om-2		
2:L:150:LYS:HG3	2:L:151:ILE:N	2.33	0.43	
2:L:196:ILE:HG12	2:L:196:ILE:H	1.58	0.43	
1:B:26:GLY:O	1:B:27:LEU:HD23	2.18	0.43	
1:I:91:PHE:CD2	1:I:92:ARG:O	2.70	0.43	
2:L:179:LYS:HB2	2:L:251:LYS:HA	2.00	0.43	
2:L:198:GLU:HG3	2:L:199:ASN:N	2.34	0.43	
1:C:79:THR:OG1	2:L:253:ASN:ND2	2.52	0.43	
2:E:150:LYS:HA	2:E:259:SER:HB2	2.00	0.43	
2:F:280:VAL:CG2	2:F:281:GLY:N	2.79	0.43	
1:I:99:MET:HG3	2:L:239:LEU:CD2	2.48	0.43	
1:B:52:THR:O	1:B:53:HIS:ND1	2.52	0.42	
2:E:264:HIS:C	2:E:265:LEU:HD23	2.39	0.42	
1:I:66:CYS:HB3	1:I:70:GLU:HB3	2.01	0.42	
2:J:197:LYS:H	2:J:202:ASN:HD21	1.67	0.42	
2:J:243:TYR:CD1	2:J:244:GLN:N	2.87	0.42	
1:G:53:HIS:CD2	2:L:218:ASP:OD2	2.71	0.42	
2:L:243:TYR:CD1	2:L:244:GLN:N	2.88	0.42	
1:C:49:ASP:HB2	1:C:60:CYS:HB3	2.01	0.42	
1:I:29:PRO:C	1:I:30:PRO:O	2.57	0.42	
1:I:67:ASP:C	1:I:68:SER:O	2.58	0.42	
2:J:243:TYR:C	2:J:243:TYR:CD1	2.92	0.42	
2:D:231:TRP:CD2	2:E:235:ALA:HA	2.53	0.42	
2:F:123:ALA:O	2:F:124:ALA:HB2	2.19	0.42	
2:L:150:LYS:NZ	2:L:173:GLU:OE2	2.53	0.42	
2:L:181:PHE:CD1	2:L:249:GLU:HG3	2.54	0.42	
1:A:50:TYR:CE2	1:A:81:ASN:HB2	2.55	0.42	
1:B:34:ILE:HG12	1:B:38:GLY:HA2	2.01	0.42	
2:F:131:GLY:O	2:F:269:ASP:HA	2.19	0.42	
1:I:50:TYR:CZ	1:I:61:LEU:HD12	2.54	0.42	
2:L:254:ASP:C	2:L:255:ARG:HG3	2.40	0.42	
2:D:194:GLU:HB2	4:D:3088:HOH:O	2.19	0.42	
1:G:108:PRO:O	1:G:109:ARG:C	2.57	0.42	
1:G:126:VAL:HG13	1:G:127:HIS:N	2.35	0.42	
1:G:21:SER:HB2	1:G:41:CYS:HB2	2.00	0.42	
1:I:102:LYS:HG3	2:L:236:GLU:OE1	2.18	0.42	
1:G:99:MET:HE1	2:J:191:ARG:HD2	1.99	0.42	
2:L:169:LEU:HG	2:L:170:ARG:N	2.34	0.42	
2:D:192:PHE:CD1	2:D:194:GLU:CG	2.86	0.42	
2:F:212:LYS:HG2	2:F:222:LEU:HD21	2.01	0.42	
1:G:104:ARG:HB2	1:G:123:ILE:HG12	2.02	0.42	
1:H:81:ASN:ND2	1:H:82:THR:H	2.18	0.42	

![](_page_28_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:161:HIS:ND1	2:K:270:HIS:CD2	2.88	0.42
2:D:169:LEU:HA	2:D:169:LEU:HD12	1.89	0.42
2:F:208:GLN:O	2:F:224:LYS:HA	2.20	0.42
1:I:50:TYR:CD2	1:I:50:TYR:C	2.93	0.42
2:J:120:GLN:OE1	2:J:120:GLN:CA	2.67	0.42
2:J:214:THR:O	2:J:216:TYR:N	2.53	0.42
2:K:243:TYR:CD1	2:K:243:TYR:C	2.92	0.42
2:K:150:LYS:HA	2:K:259:SER:HA	2.02	0.42
2:K:190:PHE:CZ	2:K:266:ILE:HD11	2.55	0.42
2:L:224:LYS:HG3	2:L:224:LYS:O	2.19	0.42
2:D:189:TYR:HD2	2:D:272:ALA:HB1	1.85	0.42
2:D:181:PHE:HB2	2:D:280:VAL:HG23	2.02	0.42
1:B:59:PHE:CD2	2:E:159:SER:HA	2.55	0.42
2:E:243:TYR:CD1	2:E:244:GLN:N	2.87	0.42
1:I:123:ILE:HD12	1:I:123:ILE:O	2.20	0.42
2:J:173:GLU:HG2	2:J:257:PHE:HB3	2.02	0.42
2:K:175:VAL:HG22	2:K:255:ARG:CG	2.48	0.42
2:K:184:ILE:O	2:K:245:GLY:HA2	2.20	0.42
1:B:92:ARG:HG3	1:B:96:SER:O	2.20	0.41
1:C:76:CYS:H	2:L:170:ARG:CZ	2.33	0.41
2:K:207:VAL:HG13	2:K:226:ALA:HB2	2.01	0.41
2:E:126:ILE:HA	2:E:162:SER:HB2	2.02	0.41
2:E:130:ARG:HG3	2:E:130:ARG:O	2.20	0.41
1:G:73:LEU:HD21	1:G:85:GLN:CD	2.40	0.41
1:G:93:GLU:CG	1:G:94:GLU:N	2.67	0.41
2:K:197:LYS:H	2:K:202:ASN:HD21	1.67	0.41
1:A:86:CYS:SG	1:A:92:ARG:CD	3.06	0.41
1:B:120:TRP:N	1:B:120:TRP:CD2	2.86	0.41
1:B:106:GLY:O	1:B:123:ILE:HD11	2.20	0.41
2:F:173:GLU:HG2	2:F:257:PHE:HB3	2.02	0.41
2:J:189:TYR:HD2	2:J:272:ALA:HB1	1.85	0.41
1:C:62:ARG:NH1	2:F:270:HIS:ND1	2.68	0.41
1:C:75:PRO:HB3	2:L:170:ARG:CD	2.22	0.41
1:G:45:LYS:O	1:G:48:GLN:HB2	2.20	0.41
1:G:53:HIS:CD2	2:L:217:PRO:HB2	2.56	0.41
2:K:156:SER:O	2:K:157:SER:O	2.39	0.41
2:K:170:ARG:O	2:K:171:ASN:HB2	2.20	0.41
1:A:44:CYS:O	1:A:78:THR:HG22	2.21	0.41
1:G:107:CYS:HB3	1:G:108:PRO:CD	2.51	0.41
2:K:174:LEU:HB2	2:K:256:ILE:HG13	2.02	0.41
2:K:198:GLU:C	2:K:200:THR:H	2.24	0.41

![](_page_29_Picture_6.jpeg)

		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:31:GLY:HA2	1:A:78:THR:O	2.21	0.41	
2:D:225:SER:HG	2:D:227:ARG:HH12	1.67	0.41	
2:D:183:TYR:O	2:D:277:ALA:HA	2.21	0.41	
2:E:130:ARG:HG2	2:E:269:ASP:OD1	2.21	0.41	
2:F:150:LYS:HG3	2:F:151:ILE:N	2.36	0.41	
1:H:63:CYS:HA	1:H:81:ASN:HD21	1.86	0.41	
2:J:189:TYR:CD2	2:J:272:ALA:HB1	2.55	0.41	
1:C:50:TYR:CZ	1:C:81:ASN:HB2	2.55	0.41	
2:F:155:GLU:OE1	2:F:161:HIS:CE1	2.74	0.41	
2:F:212:LYS:HE2	4:F:3119:HOH:O	2.19	0.41	
2:K:126:ILE:HA	2:K:162:SER:HB2	2.02	0.41	
1:B:30:PRO:HD3	1:B:54:TRP:CD1	2.55	0.41	
2:F:181:PHE:O	2:F:280:VAL:HG22	2.20	0.41	
1:G:85:GLN:CD	1:G:119:PRO:HG3	2.40	0.41	
1:H:73:LEU:HD13	1:H:85:GLN:HB3	2.03	0.41	
2:L:155:GLU:OE1	2:L:161:HIS:CE1	2.73	0.41	
2:L:127:THR:HG23	2:L:162:SER:HB3	2.02	0.41	
2:L:189:TYR:HD2	2:L:272:ALA:HB1	1.85	0.41	
2:E:190:PHE:CZ	2:E:266:ILE:HD11	2.56	0.41	
1:H:86:CYS:SG	1:H:92:ARG:HB2	2.60	0.41	
1:H:90:THR:CB	1:H:100:CYS:HB3	2.50	0.41	
2:J:196:ILE:H	2:J:196:ILE:HG13	1.41	0.41	
2:K:243:TYR:CD1	2:K:244:GLN:N	2.89	0.41	
1:A:96:SER:N	1:A:97:PRO:HD3	2.36	0.41	
1:B:64:THR:O	1:B:82:THR:HG21	2.21	0.41	
1:C:22:SER:HA	1:C:23:PRO:HD3	1.82	0.41	
2:E:174:LEU:HB2	2:E:256:ILE:HG13	2.03	0.41	
2:L:260:VAL:HG21	2:L:266:ILE:HD11	2.03	0.41	
2:J:182:TYR:O	2:J:247:ILE:HA	2.21	0.41	
2:K:161:HIS:ND1	2:K:270:HIS:CG	2.89	0.41	
1:C:50:TYR:OH	1:C:81:ASN:HB2	2.20	0.40	
1:C:77:THR:N	1:C:80:ARG:O	2.54	0.40	
2:D:121:ARG:HG2	2:F:281:GLY:HA3	2.03	0.40	
2:E:212:LYS:HA	2:E:255:ARG:O	2.21	0.40	
2:L:126:ILE:HD12	2:L:154:TRP:CB	2.51	0.40	
1:B:52:THR:HB	1:B:79:THR:O	2.22	0.40	
2:D:199:ASN:HA	4:D:3157:HOH:O	2.21	0.40	
2:D:227:ARG:CZ	2:D:242:ILE:HG12	2.52	0.40	
1:H:22:SER:O	1:H:23:PRO:C	2.59	0.40	
2:K:252:GLU:HG2	2:K:253:ASN:OD1	2.21	0.40	
2:L:209:TYR:CD1	2:L:221:LEU:HD11	2.55	0.40	

![](_page_30_Picture_6.jpeg)

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:61:LEU:HB3	2:F:132:ARG:HH11	1.86	0.40
2:D:189:TYR:CD2	2:D:272:ALA:HB1	2.56	0.40
2:D:186:SER:HB3	2:D:208:GLN:NE2	2.36	0.40
2:E:270:HIS:CD2	2:E:271:GLU:HG3	2.57	0.40
1:I:29:PRO:O	1:I:30:PRO:O	2.40	0.40
1:B:29:PRO:O	1:B:30:PRO:C	2.60	0.40
1:H:42:ILE:HD12	1:H:42:ILE:N	2.29	0.40
1:H:50:TYR:HE1	1:H:81:ASN:ND2	2.20	0.40
2:J:198:GLU:H	2:J:198:GLU:CD	2.24	0.40
2:K:122:VAL:HG13	2:K:167:LEU:CD1	2.52	0.40
1:A:28:CYS:SG	1:A:34:ILE:HA	2.62	0.40
2:E:164:LEU:HD13	2:E:168:HIS:HA	2.04	0.40
1:I:118:THR:HA	1:I:119:PRO:HD3	1.95	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic}\\ {\rm distance}~({\rm \AA}) \end{array}$	Clash overlap (Å)
4:B:3160:HOH:O	4:H:3078:HOH:O[1_554]	0.57	1.63
4:G:3053:HOH:O	4:I:3050:HOH:O[2_656]	1.19	1.01
4:B:3160:HOH:O	4:H:3105:HOH:O[1_554]	1.82	0.38
1:B:129:GLU:CG	4:H:3079:HOH:O[1_554]	1.85	0.35

## 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	86/130~(66%)	77~(90%)	6 (7%)	3(4%)	3	1
1	В	108/130~(83%)	93~(86%)	12 (11%)	3 (3%)	5	2
1	С	86/130~(66%)	61 (71%)	23 (27%)	2 (2%)	6	3
1	G	106/130~(82%)	90~(85%)	14 (13%)	2 (2%)	8	5

![](_page_31_Picture_13.jpeg)

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Н	86/130~(66%)	75 (87%)	9 (10%)	2 (2%)	6	3
1	Ι	86/130~(66%)	72 (84%)	10 (12%)	4 (5%)	2	1
2	D	148/168~(88%)	132~(89%)	13 (9%)	3(2%)	7	4
2	E	148/168~(88%)	131~(88%)	12 (8%)	5(3%)	3	1
2	F	148/168~(88%)	124~(84%)	20~(14%)	4(3%)	5	2
2	J	148/168~(88%)	132~(89%)	13 (9%)	3(2%)	7	4
2	K	148/168~(88%)	130~(88%)	13 (9%)	5(3%)	3	1
2	L	148/168~(88%)	125 (84%)	19 (13%)	4 (3%)	5	2
All	All	$1446/1788 \ (81\%)$	1242 (86%)	164 (11%)	40 (3%)	5	2

Continued from previous page...

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Е	130	ARG
2	Е	157	SER
2	Е	197	LYS
2	Е	280	VAL
1	Н	25	GLU
1	Ι	118	THR
2	Κ	130	ARG
2	Κ	157	SER
2	К	197	LYS
2	K	280	VAL
2	L	197	LYS
1	А	68	SER
1	С	80	ARG
2	D	130	ARG
2	F	280	VAL
1	Н	23	PRO
2	J	130	ARG
2	L	280	VAL
1	А	82	THR
1	В	30	PRO
1	С	50	TYR
2	F	134	ASN
1	Ι	119	PRO
2	L	134	ASN
1	A	51	SER
2	D	215	SER

![](_page_32_Picture_8.jpeg)

Mol	Chain	Res	Type
1	G	109	ARG
2	J	200	THR
1	В	113	LYS
2	D	198	GLU
1	Ι	68	SER
2	J	215	SER
2	L	153	SER
2	F	153	SER
2	F	196	ILE
1	В	96	SER
2	Е	148	GLY
1	G	119	PRO
1	Ι	30	PRO
2	K	196	ILE

#### 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	84/117~(72%)	64 (76%)	20 (24%)	0	0
1	В	97/117~(83%)	76 (78%)	21 (22%)	1	1
1	С	83/117~(71%)	62~(75%)	21~(25%)	0	0
1	G	99/117~(85%)	78 (79%)	21 (21%)	1	1
1	Η	82/117~(70%)	61~(74%)	21~(26%)	0	0
1	Ι	84/117~(72%)	60~(71%)	24 (29%)	0	0
2	D	134/149~(90%)	117~(87%)	17~(13%)	4	3
2	Ε	134/149~(90%)	111~(83%)	23~(17%)	2	1
2	F	133/149~(89%)	119~(90%)	14~(10%)	7	6
2	J	133/149~(89%)	113~(85%)	20~(15%)	3	2
2	Κ	134/149~(90%)	114~(85%)	20~(15%)	3	2
2	L	131/149~(88%)	113 (86%)	18 (14%)	3	3
All	All	1328/1596~(83%)	1088 (82%)	240 (18%)	1	1

![](_page_33_Picture_9.jpeg)

Mol	Chain	Res Type	
1	А	22	SER
1	А	24	SER
1	А	39	ARG
1	А	40	ASP
1	А	45	LYS
1	А	48	GLN
1	А	49	ASP
1	А	52	THR
1	А	58	LEU
1	А	65	ARG
1	А	66	CYS
1	А	71	VAL
1	А	73	LEU
1	A	74	SER
1	A	76	CYS
1	А	80	ARG
1	А	81	ASN
1	А	87	GLU
1	А	102	LYS
1	А	123	ILE
1	В	22	SER
1	В	24	SER
1	В	27	LEU
1	В	36	GLU
1	В	48	GLN
1	В	52	THR
1	В	58	LEU
1	В	65	ARG
1	В	68	SER
1	В	72	GLU
1	B	74	SER
1	В	82	THR
1	В	93	GLU
1	В	101	ARG
1	B	104	ARG
1	В	109	ARG
1	В	111	MET
1	В	114	VAL
1	В	118	THR
1	В	120	TRP
1	В	121	SER
1	C	22	SER

All (240) residues with a non-rotameric sidechain are listed below:

![](_page_34_Picture_6.jpeg)

Mol	Chain	Res	Type
1	С	34	ILE
1	С	39	ARG
1	С	40	ASP
1	С	49	ASP
1	С	51	SER
1	С	57	LEU
1	С	58	LEU
1	С	62	ARG
1	С	67	ASP
1	С	68	SER
1	С	73	LEU
1	С	74	SER
1	С	80	ARG
1	С	82	THR
1	С	83	VAL
1	С	92	ARG
1	С	101	ARG
1	С	116	ASP
1	С	118	THR
1	С	120	TRP
2	D	120	GLN
2	D	126	ILE
2	D	127	THR
2	D	130	ARG
2	D	132	ARG
2	D	153	SER
2	D	158	ARG
2	D	167	LEU
2	D	178	GLU
2	D	179	LYS
2	D	195	GLU
2	D	196	ILE
2	D	218	ASP
2	D	233	LYS
2	D	251	LYS
2	D	256	ILE
2	D	263	GLU
2	E	121	ARG
2	E	130	ARG
2	E	149	ARG
2	E	156	SER
2	E	157	SER

![](_page_35_Picture_6.jpeg)

Mol	Chain	Res Type		
2	Е	158	ARG	
2	Е	161	HIS	
2	Е	167	LEU	
2	Е	179	LYS	
2	Е	194	GLU	
2	Е	197	LYS	
2	Е	201	LYS	
2	Е	212	LYS	
2	Е	215	SER	
2	Е	228	ASN	
2	Е	230	CYS	
2	Е	233	LYS	
2	Е	241	SER	
2	Е	244	GLN	
2	Е	251	LYS	
2	Е	259	SER	
2	Е	274	PHE	
2	Е	280	VAL	
2	F	127	THR	
2	F	130	ARG	
2	F	133	SER	
2	F	158	ARG	
2	F	195	GLU	
2	F	215	SER	
2	F	218	ASP	
2	F	233	LYS	
2	F	234	ASP	
2	F	244	GLN	
2	F	251	LYS	
2	F	256	ILE	
2	F	263	GLU	
2	F	266	ILE	
1	G	34	ILE	
1	G	45	LYS	
1	G	52	THR	
1	G	58	LEU	
1	G	62	ARG	
1	G	67	ASP	
1	G	68	SER	
1	G	77	THR	
1	G	80	ARG	
1	G	88	GLU	

![](_page_36_Picture_6.jpeg)

Mol	Chain	Res Type		
1	G	93	GLU	
1	G	102	LYS	
1	G	105	THR	
1	G	111	MET	
1	G	116	ASP	
1	G	117	CYS	
1	G	118	THR	
1	G	121	SER	
1	G	124	GLU	
1	G	126	VAL	
1	G	128	LYS	
1	Н	24	SER	
1	Н	25	GLU	
1	H	39	ARG	
1	Н	43	SER	
1	H	45	LYS	
1	Н	49	ASP	
1	Н	51	SER	
1	Н	52	THR	
1	Н	56	ASP	
1	Н	62	ARG	
1	Н	67	ASP	
1	Н	73	LEU	
1	Н	74	SER	
1	Н	81	ASN	
1	Н	82	THR	
1	Н	88	GLU	
1	Н	93	GLU	
1	Н	116	ASP	
1	Н	117	CYS	
1	Н	120	TRP	
1	Н	121	SER	
1	I	21	SER	
1	Ι	22	SER	
1	I	34	ILE	
1	Ι	37	ASP	
1	Ι	39	ARG	
1	I	40	ASP	
1	Ι	42	ILE	
1	Ι	43	SER	
1	Ι	45	LYS	
1	Ι	52	THR	

![](_page_37_Picture_6.jpeg)

Mol	Chain	Res Type		
1	Ι	58	LEU	
1	Ι	62	ARG	
1	Ι	65	ARG	
1	Ι	67	ASP	
1	Ι	68	SER	
1	Ι	71	VAL	
1	Ι	80	ARG	
1	Ι	82	THR	
1	Ι	88	GLU	
1	Ι	92	ARG	
1	Ι	99	MET	
1	Ι	116	ASP	
1	Ι	118	THR	
1	Ι	123	ILE	
2	J	120	GLN	
2	J	126	ILE	
2	J	127	THR	
2	J	130	ARG	
2	J	132	ARG	
2	J	153	SER	
2	J	158	ARG	
2	J	167	LEU	
2	J	178	GLU	
2	J	179	LYS	
2	J	196	ILE	
2	J	199	ASN	
2	J	200	THR	
2	J	218	ASP	
2	J	224	LYS	
2	J	233	LYS	
2	J	239	LEU	
2	J	251	LYS	
2	J	256	ILE	
2	J	263	GLU	
2	K	121	ARG	
2	K	130	ARG	
2	K	149	ARG	
2	K	156	SER	
2	K	157	SER	
2	K	158	ARG	
2	K	161	HIS	
2	K	179	LYS	

![](_page_38_Picture_6.jpeg)

Mol	Chain	Res	Type	
2	K	194	GLU	
2	K	197	LYS	
2	K	201	LYS	
2	K	212	LYS	
2	K	215	SER	
2	K	233	LYS	
2	K	241	SER	
2	K	244	GLN	
2	K	251	LYS	
2	K	259	SER	
2	K	274	PHE	
2	K	280	VAL	
2	L	130	ARG	
2	L	133	SER	
2	L	152	ASN	
2	L	156	SER	
2	L	158	ARG	
2	L	194	GLU	
2	L	195	GLU	
2	L	196	ILE	
2	L	215	SER	
2	L	218	ASP	
2	L	225	SER	
2	L	233	LYS	
2	L	234	ASP	
2	L	244	GLN	
2	L	251	LYS	
2	L	256	ILE	
2	L	263	GLU	
2	L	266	ILE	

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	32	HIS
1	А	48	GLN
1	А	81	ASN
1	В	32	HIS
1	В	33	HIS
1	В	81	ASN
1	С	33	HIS
2	D	134	ASN

![](_page_39_Picture_8.jpeg)

$\overline{Mol}$	lol Chain		Type	
2	D	208	GLN	
2	D	228	ASN	
2	D	270	HIS	
2	Е	134	ASN	
2	Е	171	ASN	
2	Е	202	ASN	
2	Е	228	ASN	
2	F	161	HIS	
2	F	208	GLN	
2	F	270	HIS	
1	G	32	HIS	
1	Н	32	HIS	
1	Н	33	HIS	
1	Н	81	ASN	
1	Ι	32	HIS	
1	Ι	33	HIS	
1	Ι	48	GLN	
1	Ι	53	HIS	
2	J	202	ASN	
2	J	208	GLN	
2	J	228	ASN	
2	J	270	HIS	
2	K	134	ASN	
2	K	171	ASN	
2	K	202	ASN	
2	K	228	ASN	
2	K	270	HIS	
2	L	161	HIS	
2	L	208	GLN	
2	L	253	ASN	
2	L	270	HIS	

Continued from previous page...

### 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.

![](_page_40_Picture_9.jpeg)

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Ι	1
2	D	1
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ι	117:CYS	С	118:THR	Ν	1.82
1	D	191:ARG	С	192:PHE	Ν	1.20
1	F	191:ARG	С	192:PHE	Ν	1.12

![](_page_41_Picture_20.jpeg)

## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

![](_page_42_Picture_14.jpeg)