

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

#### Aug 17, 2023 – 04:09 PM JST

PDB ID	:	8IVW
Title	:	Crystal structure of NRP2 in complex with aNRP2-10 Fab fragment
Authors	:	Geng, Y.; Zhai, L.
Deposited on	:	2023-03-29
Resolution	:	3.21  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
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
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)	:	2.35

# 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 3.21 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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		$\mathbf{Q}_{1}$	uality of chair	ı		
1	А	583	6%	51%	19%	·	27%	_
1	D	583	9%	51%	17%	•	28%	
1	G	583	14%	46%	20%	·	31%	
1	J	583	12%	51%	17%	5%	27%	_
2	В	228	4%	63%		26%	7%	•
2	Е	228	2%	63%		25%	8%	•



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Mol	Chain	Length	Quality of chain							
			4%							
2	Н	228	64%	25%	7% •					
			2%							
2	K	228	63%	25%	7% •					
			7%							
3	С	215	60%	34%	6%					
			8%							
3	F	215	62%	33%	5%					
			5%							
3	Ι	215	60%	34%	5%					
	-		7%							
3	L	215	60%	34%	6%					



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26621 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		At	oms			ZeroOcc	AltConf	Trace
1	Λ	496	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	420	3412	2169	594	632	17	0	0	0
1	л	420	Total	С	Ν	0	S	0	0	0
	D	420	3337	2122	575	623	17	0	0	0
1	С	402	Total	С	Ν	0	S	0	0	0
	G	402	3202	2030	557	599	16	0	0	0
1	т	497	Total	С	Ν	0	S	0	0	0
	J	427	3410	2166	591	636	17	0	0	0

• Molecule 1 is a protein called Neuropilin-2.

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	13	HIS	-	expression tag	UNP O60462
А	14	HIS	-	expression tag	UNP O60462
А	15	HIS	-	expression tag	UNP O60462
A	16	HIS	-	expression tag	UNP O60462
A	17	HIS	-	expression tag	UNP O60462
A	18	HIS	-	expression tag	UNP O60462
А	19	GLU	-	expression tag	UNP O60462
А	20	ASN	-	expression tag	UNP O60462
А	21	LEU	-	expression tag	UNP O60462
А	22	TYR	-	expression tag	UNP O60462
А	23	PHE	-	expression tag	UNP O60462
А	24	GLN	-	expression tag	UNP O60462
D	13	HIS	-	expression tag	UNP O60462
D	14	HIS	-	expression tag	UNP O60462
D	15	HIS	-	expression tag	UNP O60462
D	16	HIS	-	expression tag	UNP O60462
D	17	HIS	-	expression tag	UNP O60462
D	18	HIS	-	expression tag	UNP O60462
D	19	GLU	-	expression tag	UNP O60462
D	20	ASN	-	expression tag	UNP O60462
D	21	LEU	-	expression tag	UNP O60462
				Continued	on next page



Chain	Residue	Modelled	Actual	Comment	Reference
D	22	TYR	-	expression tag	UNP O60462
D	23	PHE	-	expression tag	UNP O60462
D	24	GLN	-	expression tag	UNP O60462
G	13	HIS	-	expression tag	UNP O60462
G	14	HIS	-	expression tag	UNP O60462
G	15	HIS	-	expression tag	UNP O60462
G	16	HIS	-	expression tag	UNP O60462
G	17	HIS	-	expression tag	UNP O60462
G	18	HIS	-	expression tag	UNP O60462
G	19	GLU	-	expression tag	UNP O60462
G	20	ASN	-	expression tag	UNP O60462
G	21	LEU	-	expression tag	UNP O60462
G	22	TYR	-	expression tag	UNP O60462
G	23	PHE	-	expression tag	UNP O60462
G	24	GLN	-	expression tag	UNP O60462
J	13	HIS	-	expression tag	UNP O60462
J	14	HIS	-	expression tag	UNP O60462
J	15	HIS	-	expression tag	UNP O60462
J	16	HIS	-	expression tag	UNP O60462
J	17	HIS	-	expression tag	UNP O60462
J	18	HIS	-	expression tag	UNP O60462
J	19	GLU	-	expression tag	UNP O60462
J	20	ASN	-	expression tag	UNP O60462
J	21	LEU	-	expression tag	UNP 060462
J	22	TYR	-	expression tag	UNP 060462
J	23	PHE	-	expression tag	UNP O60462
J	24	GLN	-	expression tag	UNP O60462

• Molecule 2 is a protein called Heavy chian of antibody 10V8 Fab fragment.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	D	210	Total	С	Ν	0	S	0		
	D	219	1664	1053	273	331	7	0	0	0
0	F	220	Total	С	Ν	0	S	0	0	0
		220	1668	1055	274	332	$\overline{7}$	0	0	0
0	и	220	Total	С	Ν	0	S	0	0	0
	п	220	1668	1055	274	332	7	0	0	0
0	K	220	Total	С	Ν	0	S	0	0	0
	2 K	220	1668	1055	274	332	7		0	

• Molecule 3 is a protein called Light chain of antibody 10V8 Fab fragment.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2		215	Total	С	Ν	0	S	0 0	0	
່ງ		210	1648	1029	277	336	6	0	0	0
2	Б	215	Total	С	Ν	0	S	0	0	0
່ <u>ບ</u>	Г	215	1648	1029	277	336	6	0	0	0
2	т	215	Total	С	Ν	0	S	0	0	0
່ <u>ບ</u>	1	210	1648	1029	277	336	6	0	0	0
2	т	215	Total	С	Ν	0	S	0	0	0
່ <u>ບ</u>	3 L	215	1648	1029	277	336	6		0	



# 3 Residue-property plots (i)

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



• Molecule 1: Neuropilin-2













# 1181 1181 1186 1186 1186 1186 1187 1186 1193 1193 1193 1193 1198 1198 1198 1198 1198 1198 1198 1198 1198 1198 1198 1118 1198 1118 1198 1118 1198 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1118 1116 1118 1116 1118 1116 1118 1116 1118 1116 1118 1116 1118 1116 1118 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 1116 <t

• Molecule 3: Light chain of antibody 10V8 Fab fragment







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	70.42Å 225.16Å 143.00Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $91.30^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	49.65 - 3.21	Depositor
Resolution (A)	49.60 - 3.20	EDS
% Data completeness	90.6 (49.65-3.21)	Depositor
(in resolution range)	84.7(49.60-3.20)	EDS
R <sub>merge</sub>	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.44 (at 3.19 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
D D	0.248 , $0.294$	Depositor
$\Lambda, \Lambda_{free}$	0.249 , $0.295$	DCC
$R_{free}$ test set	3309 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	59.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $54.3$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	26621	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

Mol	Chain	Bond	lengths	Bond angles		
	Ullaili	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.36	0/3503	0.69	0/4755	
1	D	0.35	0/3426	0.67	0/4654	
1	G	0.36	0/3283	0.69	1/4452~(0.0%)	
1	J	0.35	0/3502	0.67	0/4757	
2	В	0.33	0/1705	0.72	0/2326	
2	Е	0.34	0/1709	0.72	0/2331	
2	Н	0.34	0/1709	0.74	0/2331	
2	Κ	0.34	0/1709	0.73	0/2331	
3	С	0.37	0/1686	0.74	1/2289~(0.0%)	
3	F	0.36	0/1686	0.74	0/2289	
3	Ι	0.37	0/1686	0.74	1/2289~(0.0%)	
3	L	0.37	0/1686	0.73	0/2289	
All	All	0.35	0/27290	0.71	3/37093~(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
1	D	0	1
2	В	0	1
2	Е	0	1
2	Н	0	1
2	Κ	0	1
3	F	0	1
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C	62	ARG	NE-CZ-NH1	-5.71	117.44	120.30



Control	Continueu front prettous page							
$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{a}$	
1	G	545	GLN	CB-CA-C	5.25	120.90	110.40	
3	Ι	62	ARG	NE-CZ-NH1	-5.15	117.73	120.30	

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	123	SER	Peptide
1	D	542	ARG	Sidechain
2	Е	123	SER	Peptide
3	F	18	ARG	Sidechain
2	Н	123	SER	Peptide
2	Κ	123	SER	Peptide

## 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	3412	0	3313	93	0
1	D	3337	0	3230	88	0
1	G	3202	0	3088	97	1
1	J	3410	0	3297	140	0
2	В	1664	0	1627	54	0
2	Ε	1668	0	1630	52	1
2	Н	1668	0	1630	54	0
2	Κ	1668	0	1630	60	0
3	С	1648	0	1595	53	0
3	F	1648	0	1595	51	0
3	Ι	1648	0	1595	57	0
3	L	1648	0	1595	57	0
All	All	26621	0	25825	780	1

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 15.

All (780) 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:G:443:GLY:HA2	1:G:466:ARG:NH1	1.44	1.31
1:J:449:GLN:NE2	1:J:491:ASP:O	1.71	1.24
1:J:272:LEU:CD1	1:J:279:VAL:HG21	1.69	1.20
1:A:272:LEU:CD1	1:A:279:VAL:HG21	1.71	1.17
1:J:447:ASP:HB3	1:J:462:PRO:CG	1.74	1.17
1:J:338:MET:CE	1:J:401:PRO:HB3	1.79	1.12
1:A:272:LEU:HD13	1:A:279:VAL:HG21	1.13	1.11
1:J:272:LEU:HD13	1:J:279:VAL:CG2	1.80	1.11
1:J:447:ASP:HB3	1:J:462:PRO:HG3	1.32	1.07
1:G:236:SER:OG	1:G:334:ARG:NH2	1.86	1.07
1:D:447:ASP:OD1	1:D:462:PRO:HG2	1.55	1.06
1:J:545:GLN:HB3	1:J:546:PRO:HD2	1.35	1.05
1:J:338:MET:HE1	1:J:401:PRO:HB3	1.08	1.04
1:D:440:MET:O	1:D:466:ARG:HG2	1.60	1.02
1:A:272:LEU:HD13	1:A:279:VAL:CG2	1.89	1.02
1:J:540:ASP:O	1:J:544:GLN:N	1.94	1.00
1:J:338:MET:HE1	1:J:401:PRO:CB	1.92	1.00
1:A:471:ARG:HA	1:A:507:ARG:NE	1.77	0.99
1:J:185:MET:CE	1:J:268:HIS:HA	1.94	0.98
1:J:545:GLN:HB3	1:J:546:PRO:CD	1.92	0.98
1:J:185:MET:CE	1:J:268:HIS:CD2	2.48	0.96
1:G:443:GLY:HA2	1:G:466:ARG:HH12	1.22	0.95
1:J:445:ILE:O	1:J:466:ARG:NH2	2.00	0.95
1:J:272:LEU:HD13	1:J:279:VAL:HG21	0.95	0.95
1:D:540:ASP:O	1:D:544:GLN:N	1.99	0.94
1:A:338:MET:CE	1:A:401:PRO:HB3	1.97	0.94
1:J:545:GLN:HE21	1:J:545:GLN:HA	1.33	0.94
1:D:447:ASP:CG	1:D:462:PRO:HG2	1.87	0.94
1:J:185:MET:HE3	1:J:268:HIS:CD2	2.03	0.94
1:J:456:GLN:HA	1:J:477:ARG:HA	1.50	0.94
1:G:445:ILE:HG23	1:G:449:GLN:HE21	1.33	0.94
1:G:443:GLY:HA2	1:G:466:ARG:HH11	1.31	0.93
1:D:547:LYS:HE2	1:D:549:PHE:CE1	2.02	0.93
1:J:440:MET:O	1:J:466:ARG:HG2	1.69	0.91
1:J:185:MET:HE2	1:J:268:HIS:HA	1.53	0.89
2:K:135:CYS:SG	3:L:214:GLU:OE1	2.31	0.88
1:G:443:GLY:CA	1:G:466:ARG:NH1	2.36	0.87
1:A:185:MET:CE	1:A:268:HIS:CD2	2.59	0.86
1:D:190:GLN:HG2	1:D:237:GLU:HG2	1.54	0.86
2:K:208:HIS:NE2	2:K:210:PRO:HG2	1.91	0.85
2:E:208:HIS:NE2	2:E:210:PRO:HG2	1.91	0.85
2:B:208:HIS:CE1	2:B:210:PRO:HG2	2.11	0.85



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:338:MET:HE1	1:D:401:PRO:HB3	1.58	0.85
2:E:208:HIS:CE1	2:E:210:PRO:HG2	2.11	0.85
2:K:208:HIS:CE1	2:K:210:PRO:HG2	2.11	0.85
1:A:338:MET:HE2	1:A:401:PRO:HB3	1.58	0.85
2:H:208:HIS:NE2	2:H:210:PRO:HG2	1.91	0.85
1:J:528:TYR:CG	1:J:566:ILE:HG21	2.12	0.85
2:H:208:HIS:CE1	2:H:210:PRO:HG2	2.11	0.84
1:J:185:MET:HE2	1:J:268:HIS:CA	2.07	0.84
1:A:185:MET:HE1	1:A:268:HIS:HD2	1.41	0.84
2:B:208:HIS:NE2	2:B:210:PRO:HG2	1.91	0.83
1:G:449:GLN:NE2	1:G:491:ASP:O	2.11	0.83
1:D:445:ILE:O	1:D:466:ARG:NH2	2.11	0.82
3:F:6:GLN:HE22	3:F:88:TYR:HA	1.43	0.82
1:J:528:TYR:CZ	1:J:566:ILE:HG12	2.14	0.82
1:J:185:MET:HE1	1:J:268:HIS:CD2	2.13	0.82
1:D:539:GLN:HA	1:D:545:GLN:O	1.80	0.81
3:L:6:GLN:HE22	3:L:88:TYR:HA	1.44	0.81
3:I:6:GLN:HE22	3:I:88:TYR:HA	1.43	0.81
3:F:148:GLN:HB3	3:F:196:GLU:HB2	1.63	0.81
1:J:440:MET:O	1:J:466:ARG:NH1	2.13	0.81
1:A:449:GLN:NE2	1:A:491:ASP:O	2.14	0.81
3:L:148:GLN:HB3	3:L:196:GLU:HB2	1.63	0.81
1:D:540:ASP:O	1:D:544:GLN:CA	2.27	0.81
3:C:6:GLN:HE22	3:C:88:TYR:HA	1.43	0.81
1:A:471:ARG:HA	1:A:507:ARG:HE	1.46	0.80
1:A:185:MET:HE1	1:A:268:HIS:CD2	2.16	0.80
1:G:539:GLN:HA	1:G:546:PRO:HA	1.62	0.80
1:A:322:LEU:HD13	2:E:164:SER:HB2	1.64	0.79
1:J:375:TYR:CE1	1:J:402:LEU:CD1	2.65	0.78
1:A:161:GLU:HG3	1:A:165:PHE:HB3	1.66	0.78
3:I:148:GLN:HB3	3:I:196:GLU:HB2	1.64	0.78
1:J:471:ARG:HG2	1:J:471:ARG:HH11	1.46	0.78
1:G:161:GLU:HG3	1:G:165:PHE:HB3	1.66	0.78
1:J:528:TYR:CD2	1:J:566:ILE:CG2	2.67	0.78
2:K:189:VAL:HG11	3:L:136:LEU:HD13	1.66	0.78
1:J:185:MET:HE3	1:J:268:HIS:HA	1.65	0.78
3:C:148:GLN:HB3	3:C:196:GLU:HB2	1.64	0.78
1:J:161:GLU:HG3	1:J:165:PHE:HB3	1.66	0.77
2:H:189:VAL:HG11	3:I:136:LEU:HD13	1.67	0.77
1:J:185:MET:CE	1:J:268:HIS:CA	2.63	0.77
1:D:161:GLU:HG3	1:D:165:PHE:HB3	1.66	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:350:ARG:HG2	1:G:350:ARG:HH11	1.49	0.77
1:A:518:ARG:HG2	1:A:555:TYR:CD2	2.21	0.76
1:D:540:ASP:O	1:D:544:GLN:HA	1.85	0.76
3:F:168:ASP:HB3	3:F:171:ASP:O	1.86	0.76
3:I:168:ASP:HB3	3:I:171:ASP:O	1.85	0.76
1:J:466:ARG:HG2	1:J:466:ARG:HH11	1.49	0.76
1:A:437:MET:HE3	1:A:588:GLU:HG2	1.68	0.76
1:J:447:ASP:HB3	1:J:462:PRO:HG2	1.68	0.76
1:J:450:ILE:HD12	1:J:462:PRO:O	1.86	0.76
1:G:377:HIS:HB2	1:G:382:LYS:HB2	1.68	0.76
3:L:168:ASP:HB3	3:L:171:ASP:O	1.86	0.75
1:J:185:MET:HE1	1:J:268:HIS:HD2	1.49	0.75
1:J:518:ARG:HG2	1:J:555:TYR:CD2	2.22	0.75
1:A:360:SER:HG	1:A:413:THR:HG1	1.34	0.75
1:A:440:MET:SD	1:A:450:ILE:HD13	2.27	0.75
3:C:168:ASP:HB3	3:C:171:ASP:O	1.86	0.75
1:J:528:TYR:CD2	1:J:566:ILE:HG21	2.23	0.74
1:A:434:CYS:HB3	1:A:499:LYS:HD3	1.68	0.74
1:J:437:MET:HE3	1:J:588:GLU:HG2	1.68	0.74
1:J:545:GLN:HA	1:J:545:GLN:NE2	2.02	0.74
1:D:518:ARG:HG2	1:D:555:TYR:CD2	2.22	0.74
1:D:437:MET:HE3	1:D:588:GLU:HG2	1.69	0.74
1:G:443:GLY:CA	1:G:466:ARG:HH12	1.98	0.74
1:G:545:GLN:HB3	1:G:546:PRO:CD	2.18	0.74
2:H:2:VAL:HG22	2:H:27:PHE:HB2	1.70	0.74
1:G:564:ASP:N	1:G:564:ASP:OD1	2.13	0.74
1:J:437:MET:CE	1:J:588:GLU:HG2	2.18	0.74
2:B:2:VAL:HG22	2:B:27:PHE:HB2	1.70	0.73
1:J:540:ASP:O	1:J:544:GLN:CA	2.36	0.73
1:D:338:MET:HE1	1:D:401:PRO:CB	2.19	0.73
1:A:338:MET:HE1	1:A:401:PRO:HB3	1.68	0.73
1:D:466:ARG:HG2	1:D:466:ARG:HH11	1.54	0.72
1:A:272:LEU:HD12	1:A:279:VAL:HG21	1.66	0.72
1:G:467:LEU:HA	1:G:586:ARG:HB3	1.70	0.72
1:G:223:GLY:HA2	1:G:469:SER:OG	1.90	0.72
2:E:39:GLN:NE2	3:F:39:GLN:HE22	1.87	0.72
1:D:338:MET:CE	1:D:401:PRO:HB3	2.18	0.72
1:J:181:ALA:HB2	1:J:266:LEU:HD22	1.70	0.72
2:E:2:VAL:HG22	2:E:27:PHE:HB2	1.71	0.72
1:G:434:CYS:HB3	1:G:499:LYS:HD3	1.70	0.72
2:H:135:CYS:SG	3:I:214:GLU:OE1	2.47	0.72



	to de pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:434:CYS:HB3	1:J:499:LYS:HD3	1.72	0.72
1:A:437:MET:CE	1:A:588:GLU:HG2	2.20	0.71
2:E:60:TYR:HE1	2:E:70:ILE:HG13	1.56	0.71
2:H:60:TYR:HE1	2:H:70:ILE:HG13	1.56	0.71
1:D:434:CYS:HB3	1:D:499:LYS:HD3	1.72	0.71
2:B:60:TYR:HE1	2:B:70:ILE:HG13	1.56	0.71
1:D:181:ALA:HB2	1:D:266:LEU:HD22	1.72	0.71
1:D:437:MET:CE	1:D:588:GLU:HG2	2.20	0.71
1:G:437:MET:CE	1:G:588:GLU:HG2	2.20	0.71
1:G:354:ASN:OD1	2:H:50:ARG:NH1	2.24	0.70
2:K:2:VAL:HG22	2:K:27:PHE:HB2	1.73	0.70
1:G:452:ALA:CB	1:G:474:TRP:HE1	2.05	0.70
1:D:374:VAL:HG11	1:D:381:HIS:CD2	2.25	0.70
1:G:472:SER:O	1:G:586:ARG:HD3	1.93	0.69
1:A:338:MET:CE	1:A:401:PRO:CB	2.69	0.69
2:B:105:GLU:HA	3:C:33:TYR:CE1	2.28	0.69
3:I:136:LEU:C	3:I:137:LEU:HD23	2.13	0.69
1:A:297:SER:OG	1:A:327:GLU:OE1	2.11	0.69
2:B:164:SER:HB2	1:D:322:LEU:HD13	1.74	0.69
1:G:492:LEU:HB2	1:G:569:GLN:HG3	1.75	0.69
2:H:11:VAL:HB	2:H:155:PRO:HG3	1.75	0.69
1:J:185:MET:HE3	1:J:268:HIS:CG	2.27	0.69
2:K:105:GLU:HA	3:L:33:TYR:CE1	2.28	0.69
3:C:136:LEU:C	3:C:137:LEU:HD23	2.13	0.68
3:F:136:LEU:C	3:F:137:LEU:HD23	2.13	0.68
2:K:60:TYR:HE1	2:K:70:ILE:HG13	1.59	0.68
2:H:208:HIS:C	2:H:210:PRO:CD	2.62	0.68
1:G:191:PHE:HB2	1:G:234:THR:HG23	1.75	0.68
1:J:185:MET:CE	1:J:268:HIS:CG	2.77	0.68
1:J:542:ARG:CD	1:J:542:ARG:H	2.07	0.68
1:J:447:ASP:CB	1:J:462:PRO:CG	2.65	0.68
1:J:540:ASP:O	1:J:544:GLN:HA	1.93	0.68
2:K:39:GLN:NE2	3:L:39:GLN:HE22	1.91	0.68
1:J:545:GLN:CB	1:J:546:PRO:CD	2.70	0.67
2:B:208:HIS:C	2:B:210:PRO:CD	2.63	0.67
2:E:208:HIS:C	2:E:210:PRO:CD	2.63	0.67
3:L:136:LEU:C	3:L:137:LEU:HD23	2.14	0.67
2:K:208:HIS:C	2:K:210:PRO:CD	2.63	0.67
1:G:445:ILE:HG23	1:G:449:GLN:NE2	2.06	0.67
3:I:137:LEU:HD11	3:I:147:VAL:HG13	1.76	0.67
1:A:447:ASP:HB2	1:A:462:PRO:HG3	1.76	0.67



	io ao pago	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:209:LYS:N	2:H:210:PRO:HD3	2.10	0.66
1:J:456:GLN:HB2	1:J:476:PRO:O	1.94	0.66
1:J:528:TYR:CD2	1:J:566:ILE:HG23	2.29	0.66
2:K:105:GLU:HA	3:L:33:TYR:HE1	1.59	0.66
1:A:471:ARG:HA	1:A:507:ARG:CZ	2.25	0.66
2:B:91:THR:HG22	2:B:119:VAL:H	1.59	0.66
1:A:338:MET:HE1	1:A:401:PRO:CB	2.25	0.66
2:B:105:GLU:HA	3:C:33:TYR:HE1	1.60	0.66
2:B:208:HIS:C	2:B:210:PRO:HD2	2.16	0.66
1:D:190:GLN:NE2	1:D:237:GLU:OE2	2.28	0.66
2:E:91:THR:HG22	2:E:119:VAL:H	1.61	0.66
1:A:445:ILE:O	1:A:466:ARG:NH1	2.28	0.66
2:H:91:THR:HG22	2:H:119:VAL:H	1.60	0.66
3:C:137:LEU:HD11	3:C:147:VAL:HG13	1.77	0.66
3:C:137:LEU:HD23	3:C:137:LEU:N	2.10	0.66
2:B:189:VAL:HG11	3:C:136:LEU:HD13	1.78	0.65
2:H:209:LYS:N	2:H:210:PRO:CD	2.60	0.65
2:K:91:THR:HG22	2:K:119:VAL:H	1.61	0.65
1:J:214:ASP:HB2	1:J:248:THR:OG1	1.96	0.65
2:E:208:HIS:C	2:E:210:PRO:HD2	2.16	0.65
3:F:137:LEU:HD23	3:F:137:LEU:N	2.11	0.65
2:K:208:HIS:C	2:K:210:PRO:HD2	2.16	0.65
2:H:208:HIS:C	2:H:210:PRO:HD2	2.16	0.65
2:K:208:HIS:CG	2:K:210:PRO:HD2	2.32	0.65
1:D:214:ASP:HB2	1:D:248:THR:OG1	1.97	0.65
1:G:214:ASP:HB2	1:G:248:THR:OG1	1.97	0.65
1:A:214:ASP:HB2	1:A:248:THR:OG1	1.97	0.65
2:E:135:CYS:SG	3:F:214:GLU:OE1	2.54	0.65
3:I:137:LEU:HD23	3:I:137:LEU:N	2.10	0.65
1:D:547:LYS:HE2	1:D:549:PHE:CD1	2.32	0.65
3:L:137:LEU:HD23	3:L:137:LEU:N	2.11	0.65
3:L:137:LEU:HD11	3:L:147:VAL:HG13	1.79	0.65
2:E:208:HIS:CG	2:E:210:PRO:HD2	2.33	0.64
2:H:105:GLU:HA	3:I:33:TYR:CE1	2.32	0.64
3:F:137:LEU:HD11	3:F:147:VAL:HG13	1.78	0.64
2:K:17:THR:HG22	2:K:84:SER:HA	1.78	0.64
2:B:208:HIS:CG	2:B:210:PRO:HD2	2.32	0.64
2:B:209:LYS:N	2:B:210:PRO:CD	2.60	0.64
2:K:209:LYS:N	2:K:210:PRO:HD3	2.12	0.64
2:K:209:LYS:N	2:K:210:PRO:CD	2.60	0.64
1:J:440:MET:O	1:J:466:ARG:CG	2.45	0.64



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:209:LYS:N	2:B:210:PRO:HD3	2.12	0.64
2:E:189:VAL:HG11	3:F:136:LEU:HD13	1.78	0.64
2:E:209:LYS:N	2:E:210:PRO:CD	2.60	0.64
2:E:209:LYS:N	2:E:210:PRO:HD3	2.12	0.64
1:J:542:ARG:H	1:J:542:ARG:HD3	1.62	0.64
1:D:449:GLN:NE2	1:D:491:ASP:O	2.31	0.64
1:D:518:ARG:HG2	1:D:555:TYR:CG	2.32	0.64
1:J:518:ARG:HG2	1:J:555:TYR:CG	2.32	0.64
1:J:301:ASP:OD1	1:J:303:ARG:N	2.31	0.63
2:B:17:THR:HG22	2:B:84:SER:HA	1.79	0.63
2:E:17:THR:HG22	2:E:84:SER:HA	1.79	0.63
1:G:358:VAL:HG13	1:G:411:PRO:HB3	1.79	0.63
2:H:17:THR:HG22	2:H:84:SER:HA	1.80	0.63
1:J:375:TYR:CE1	1:J:402:LEU:HD11	2.33	0.63
2:K:42:GLY:O	2:K:43:LYS:HB2	1.98	0.63
1:A:518:ARG:HG2	1:A:555:TYR:CG	2.34	0.63
3:F:62:ARG:NH1	3:F:80:GLN:HB2	2.14	0.63
1:A:185:MET:CE	1:A:268:HIS:HD2	2.01	0.62
1:D:178:THR:HG22	1:D:180:LEU:CD2	2.29	0.62
1:D:338:MET:SD	1:D:403:LEU:CD1	2.87	0.62
2:E:105:GLU:HA	3:F:33:TYR:CE1	2.34	0.62
2:H:105:GLU:HA	3:I:33:TYR:HE1	1.64	0.62
1:J:375:TYR:CD1	1:J:402:LEU:HD11	2.33	0.62
1:J:447:ASP:CB	1:J:462:PRO:HG3	2.20	0.62
1:D:374:VAL:CG1	1:D:381:HIS:CD2	2.82	0.62
2:H:208:HIS:CG	2:H:210:PRO:HD2	2.34	0.62
3:L:62:ARG:NH1	3:L:80:GLN:HB2	2.15	0.62
3:C:62:ARG:NH1	3:C:80:GLN:HB2	2.14	0.61
2:B:42:GLY:O	2:B:43:LYS:HB2	1.98	0.61
1:G:208:CYS:HB2	1:G:228:LYS:HD3	1.82	0.61
1:G:437:MET:HE3	1:G:588:GLU:HG2	1.81	0.61
1:G:399:HIS:CD2	1:G:399:HIS:H	2.18	0.61
2:H:189:VAL:HG11	3:I:136:LEU:CD1	2.30	0.61
3:I:62:ARG:NH1	3:I:80:GLN:HB2	2.15	0.61
1:J:338:MET:SD	1:J:403:LEU:CD1	2.89	0.61
1:D:538:ILE:O	1:D:546:PRO:HA	2.01	0.61
1:J:543:THR:HG22	1:J:545:GLN:HB2	1.82	0.61
2:E:42:GLY:O	2:E:43:LYS:HB2	1.99	0.60
2:B:88:SER:O	2:B:91:THR:HG23	2.01	0.60
2:E:105:GLU:HA	3:F:33:TYR:HE1	1.65	0.60
2:K:189:VAL:HG11	3:L:136:LEU:CD1	2.31	0.60



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:208:CYS:HB2	1:D:228:LYS:HD3	1.83	0.60
1:J:208:CYS:HB2	1:J:228:LYS:HD3	1.84	0.60
1:J:323:ASP:OD2	2:K:104:ARG:NH2	2.34	0.60
1:J:443:GLY:HA2	1:J:466:ARG:NH1	2.17	0.60
1:G:545:GLN:HB3	1:G:546:PRO:HD2	1.82	0.60
2:H:42:GLY:O	2:H:43:LYS:HB2	1.99	0.60
2:K:88:SER:O	2:K:91:THR:HG23	2.01	0.60
1:A:338:MET:HE2	1:A:401:PRO:CB	2.31	0.60
2:B:135:CYS:SG	3:C:214:GLU:OE1	2.58	0.60
1:G:288:ILE:O	1:G:310:ARG:NH1	2.35	0.60
1:G:350:ARG:HG2	1:G:350:ARG:NH1	2.17	0.60
1:A:288:ILE:O	1:A:310:ARG:NH1	2.35	0.59
2:E:88:SER:O	2:E:91:THR:HG23	2.02	0.59
1:G:358:VAL:HG21	1:G:420:LEU:HD13	1.83	0.59
2:H:88:SER:O	2:H:91:THR:HG23	2.01	0.59
1:J:185:MET:CE	1:J:268:HIS:CB	2.81	0.59
1:D:443:GLY:HA2	1:D:466:ARG:NH1	2.17	0.59
1:D:288:ILE:O	1:D:310:ARG:NH1	2.35	0.59
2:K:43:LYS:HE3	3:L:86:THR:HG21	1.84	0.59
2:B:11:VAL:HB	2:B:155:PRO:HG3	1.85	0.59
1:J:288:ILE:O	1:J:310:ARG:NH1	2.35	0.58
1:G:474:TRP:HZ3	1:G:583:ILE:CG2	2.17	0.58
1:A:208:CYS:HB2	1:A:228:LYS:HD3	1.84	0.58
2:H:208:HIS:NE2	2:H:210:PRO:CG	2.66	0.58
1:J:528:TYR:CE1	1:J:566:ILE:HG12	2.38	0.58
3:C:62:ARG:HH12	3:C:80:GLN:HB2	1.69	0.58
2:H:43:LYS:HE3	3:I:86:THR:HG21	1.86	0.58
1:A:342:ILE:HD11	1:A:363:LEU:HD22	1.84	0.58
1:G:447:ASP:HA	1:G:450:ILE:HD12	1.85	0.58
1:G:525:LYS:HG2	1:G:547:LYS:O	2.04	0.57
1:J:456:GLN:HA	1:J:477:ARG:CA	2.28	0.57
2:K:52:ASP:HB3	2:K:55:ASP:O	2.04	0.57
2:E:30:LYS:HE2	2:E:74:THR:HG21	1.86	0.57
1:D:186:GLU:HG2	1:D:240:SER:O	2.05	0.57
1:D:457:GLU:N	1:D:457:GLU:OE1	2.37	0.57
1:G:474:TRP:HZ3	1:G:583:ILE:HG22	1.68	0.57
1:J:375:TYR:HE1	1:J:402:LEU:CD1	2.18	0.57
2:K:208:HIS:NE2	2:K:210:PRO:CG	2.66	0.57
2:H:52:ASP:HB3	2:H:55:ASP:O	2.04	0.57
2:E:52:ASP:HB3	2:E:55:ASP:O	2.05	0.56
2:E:208:HIS:NE2	2:E:210:PRO:CG	2.66	0.56



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:I:62:ARG:HH12	3:I:80:GLN:HB2	1.71	0.56	
1:J:463:SER:HA	1:J:466:ARG:HD2	1.87	0.56	
3:L:2:ILE:HD11	3:L:29:VAL:HG22	1.87	0.56	
1:A:178:THR:HG22	1:A:180:LEU:HD22	1.87	0.56	
1:A:178:THR:HG22	1:A:180:LEU:CD2	2.35	0.56	
1:A:537:TYR:HB3	1:A:546:PRO:HB3	1.86	0.56	
2:B:52:ASP:HB3	2:B:55:ASP:O	2.05	0.56	
1:J:466:ARG:HG2	1:J:466:ARG:NH1	2.20	0.56	
1:J:171:HIS:HB3	1:J:253:MET:HA	1.87	0.56	
1:D:338:MET:HG2	1:D:403:LEU:HD11	1.86	0.56	
1:A:171:HIS:HB3	1:A:253:MET:HA	1.88	0.56	
1:A:440:MET:SD	1:A:450:ILE:CD1	2.94	0.56	
1:G:171:HIS:HB3	1:G:253:MET:HA	1.87	0.56	
2:H:202:TYR:H	2:H:220:GLY:HA2	1.70	0.56	
1:J:445:ILE:HD13	1:J:490:VAL:HG13	1.88	0.56	
1:D:169:TYR:CE2	1:D:257:LYS:HB2	2.41	0.56	
1:D:171:HIS:HB3	1:D:253:MET:HA	1.87	0.56	
1:J:169:TYR:CE2	1:J:257:LYS:HB2	2.41	0.56	
1:A:456:GLN:HA	1:A:477:ARG:HA	1.87	0.55	
2:E:60:TYR:CE1	2:E:70:ILE:HG13	2.41	0.55	
3:C:3:GLN:HG2	3:C:26:SER:HB3	1.88	0.55	
2:E:202:TYR:H	2:E:220:GLY:HA2	1.71	0.55	
3:F:62:ARG:HH12	3:F:80:GLN:HB2	1.70	0.55	
1:J:365:VAL:HG21	1:J:402:LEU:CD2	2.35	0.55	
1:D:365:VAL:HG21	1:D:402:LEU:HD21	1.88	0.55	
1:D:539:GLN:OE1	1:D:545:GLN:HA	2.06	0.55	
3:L:3:GLN:HG2	3:L:26:SER:HB3	1.88	0.55	
1:G:360:SER:HG	1:G:413:THR:HG1	1.54	0.55	
1:G:467:LEU:O	1:G:467:LEU:HD23	2.06	0.55	
1:J:375:TYR:CD1	1:J:402:LEU:CD1	2.89	0.55	
2:H:43:LYS:NZ	3:I:101:GLY:O	2.34	0.55	
1:J:467:LEU:HD12	1:J:504:GLN:OE1	2.07	0.55	
2:B:208:HIS:NE2	2:B:210:PRO:CG	2.66	0.55	
1:J:453:SER:HB3	1:J:487:TRP:CD1	2.42	0.55	
1:G:169:TYR:CE2	1:G:257:LYS:HB2	2.41	0.55	
2:H:39:GLN:NE2	3:I:39:GLN:HE22	2.05	0.55	
2:H:87:ARG:HG2	1:J:350:ARG:HH21	1.69	0.55	
2:B:32:TYR:HD1	2:B:32:TYR:H	1.54	0.55	
1:D:158:GLY:HA3	1:D:264:TYR:CE2	2.42	0.55	
1:J:443:GLY:HA2	1:J:466:ARG:HH12	1.71	0.55	
1:D:186:GLU:HG3	1:D:241:SER:HB3	1.89	0.55	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:105:GLU:OE1	3:L:51:ARG:NE	2.40	0.55
3:L:7:SER:HB3	3:L:22:THR:OG1	2.07	0.55
1:A:169:TYR:CE2	1:A:257:LYS:HB2	2.41	0.55
3:F:3:GLN:HG2	3:F:26:SER:HB3	1.88	0.54
1:G:222:VAL:HG11	1:G:466:ARG:NH1	2.22	0.54
1:G:445:ILE:HG22	1:G:445:ILE:O	2.07	0.54
2:H:20:ILE:HG21	2:H:115:THR:HG21	1.89	0.54
1:J:445:ILE:HD13	1:J:490:VAL:CG1	2.37	0.54
2:K:11:VAL:HB	2:K:155:PRO:HG3	1.87	0.54
2:K:202:TYR:H	2:K:220:GLY:HA2	1.72	0.54
1:J:158:GLY:HA3	1:J:264:TYR:CE2	2.43	0.54
2:B:20:ILE:HG21	2:B:115:THR:HG21	1.90	0.54
1:G:222:VAL:CG1	1:G:466:ARG:CZ	2.86	0.54
1:G:229:TYR:CZ	1:G:235:PRO:HB3	2.43	0.54
1:J:181:ALA:CB	1:J:266:LEU:HD22	2.36	0.54
2:K:189:VAL:HG13	3:L:136:LEU:HD11	1.89	0.54
3:F:7:SER:HB3	3:F:22:THR:OG1	2.08	0.54
2:H:32:TYR:HD1	2:H:32:TYR:H	1.54	0.54
3:L:62:ARG:HH12	3:L:80:GLN:HB2	1.71	0.54
1:A:471:ARG:HB3	1:A:507:ARG:CZ	2.37	0.54
2:E:32:TYR:HD1	2:E:32:TYR:H	1.55	0.54
3:I:2:ILE:HD11	3:I:29:VAL:HG22	1.88	0.54
3:I:7:SER:HB3	3:I:22:THR:OG1	2.07	0.54
1:J:531:ASN:HB3	1:J:533:LYS:HG3	1.89	0.54
2:B:18:VAL:CG2	2:B:86:LEU:HD11	2.39	0.53
1:G:158:GLY:HA3	1:G:264:TYR:CE2	2.43	0.53
1:D:466:ARG:HH11	1:D:466:ARG:CG	2.21	0.53
2:H:164:SER:HA	2:H:205:ASN:OD1	2.08	0.53
3:L:8:PRO:HB2	3:L:11:LEU:CD1	2.38	0.53
1:A:440:MET:CE	1:A:450:ILE:HD13	2.38	0.53
2:B:39:GLN:NE2	3:C:39:GLN:HE22	2.07	0.53
3:C:21:ILE:HD12	3:C:74:LEU:HD23	1.91	0.53
3:F:2:ILE:HD11	3:F:29:VAL:HG22	1.89	0.53
3:F:21:ILE:HD12	3:F:74:LEU:HD23	1.90	0.53
1:G:363:LEU:HD23	1:G:375:TYR:HB2	1.91	0.53
1:A:158:GLY:HA3	1:A:264:TYR:CE2	2.43	0.53
1:A:531:ASN:HB3	1:A:533:LYS:HG3	1.91	0.53
1:D:531:ASN:HB3	1:D:533:LYS:HG3	1.89	0.53
1:J:539:GLN:H	1:J:539:GLN:HE21	1.56	0.53
2:K:60:TYR:CE1	2:K:70:ILE:HG13	2.43	0.53
2:K:18:VAL:CG2	2:K:86:LEU:HD11	2.39	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:3:GLN:HG2	3:I:26:SER:HB3	1.90	0.53
1:A:528:TYR:CZ	1:A:566:ILE:HG12	2.44	0.53
3:C:7:SER:HB3	3:C:22:THR:OG1	2.08	0.53
1:J:272:LEU:HD12	1:J:279:VAL:HG21	1.81	0.53
2:K:20:ILE:HG21	2:K:115:THR:HG21	1.91	0.53
3:L:21:ILE:HD12	3:L:74:LEU:HD23	1.91	0.53
1:A:447:ASP:HB2	1:A:462:PRO:CG	2.39	0.52
2:E:20:ILE:HG21	2:E:115:THR:HG21	1.92	0.52
2:H:189:VAL:HG13	3:I:136:LEU:HD11	1.91	0.52
2:B:164:SER:HA	2:B:205:ASN:OD1	2.09	0.52
1:A:344:THR:C	1:A:387:ASN:HD21	2.13	0.52
1:D:500:GLY:HA2	1:D:563:PHE:CE2	2.45	0.52
1:G:435:SER:OG	1:G:562:ARG:NH2	2.41	0.52
2:K:189:VAL:CG1	3:L:136:LEU:CD1	2.87	0.52
2:E:11:VAL:HB	2:E:155:PRO:HG3	1.91	0.52
2:H:18:VAL:CG2	2:H:86:LEU:HD11	2.40	0.52
3:I:21:ILE:HD12	3:I:74:LEU:HD23	1.92	0.52
1:J:447:ASP:OD1	1:J:447:ASP:N	2.42	0.52
2:K:32:TYR:H	2:K:32:TYR:HD1	1.56	0.52
3:L:8:PRO:HB2	3:L:11:LEU:HD11	1.91	0.52
1:A:500:GLY:HA2	1:A:563:PHE:CE2	2.44	0.52
2:B:189:VAL:HG11	3:C:136:LEU:CD1	2.38	0.52
2:E:18:VAL:CG2	2:E:86:LEU:HD11	2.40	0.52
2:E:164:SER:HA	2:E:205:ASN:OD1	2.09	0.52
1:G:500:GLY:HA2	1:G:563:PHE:CE2	2.44	0.52
1:D:323:ASP:OD2	2:E:104:ARG:NH2	2.43	0.52
1:D:454:SER:HB3	1:D:486:GLU:OE1	2.10	0.52
1:G:222:VAL:CG1	1:G:466:ARG:NH1	2.73	0.52
1:J:471:ARG:NH1	1:J:471:ARG:CG	2.73	0.52
2:B:51:ILE:HD12	2:B:58:THR:HG22	1.92	0.52
3:I:8:PRO:HB2	3:I:11:LEU:HD11	1.92	0.52
1:J:500:GLY:HA2	1:J:563:PHE:CE2	2.45	0.52
3:F:8:PRO:HB2	3:F:11:LEU:CD1	2.41	0.51
1:G:290:ASN:OD1	1:G:310:ARG:NH2	2.44	0.51
3:C:2:ILE:HD11	3:C:29:VAL:HG22	1.90	0.51
2:H:60:TYR:CE1	2:H:70:ILE:HG13	2.41	0.51
2:K:164:SER:HA	2:K:205:ASN:OD1	2.09	0.51
1:A:290:ASN:OD1	1:A:310:ARG:NH2	2.43	0.51
1:J:542:ARG:CD	1:J:542:ARG:N	2.73	0.51
1:D:567:PRO:HB2	1:D:594:TRP:HZ2	1.75	0.51
1:G:350:ARG:HH21	2:K:87:ARG:HG2	1.75	0.51



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:189:VAL:CG1	3:I:136:LEU:CD1	2.88	0.51
1:D:290:ASN:OD1	1:D:310:ARG:NH2	2.43	0.51
1:J:471:ARG:HG2	1:J:471:ARG:NH1	2.19	0.51
1:G:480:GLN:OE1	1:G:480:GLN:HA	2.10	0.51
1:G:543:THR:O	1:G:545:GLN:N	2.44	0.51
1:J:185:MET:HE2	1:J:268:HIS:N	2.25	0.51
1:A:480:GLN:HA	1:A:480:GLN:OE1	2.11	0.51
2:B:130:PHE:CE2	3:C:125:GLN:HG3	2.45	0.51
1:D:185:MET:HA	1:D:185:MET:CE	2.41	0.51
1:D:435:SER:OG	1:D:562:ARG:NH2	2.42	0.51
1:J:290:ASN:OD1	1:J:310:ARG:NH2	2.44	0.51
2:B:208:HIS:CD2	2:B:210:PRO:CG	2.94	0.51
1:D:181:ALA:CB	1:D:266:LEU:HD22	2.40	0.51
2:B:60:TYR:CE1	2:B:70:ILE:HG13	2.41	0.51
1:D:178:THR:HG22	1:D:180:LEU:HD22	1.92	0.50
2:H:208:HIS:CD2	2:H:210:PRO:CG	2.94	0.50
2:K:208:HIS:CD2	2:K:210:PRO:CG	2.94	0.50
2:B:91:THR:HG22	2:B:119:VAL:N	2.26	0.50
1:D:186:GLU:HG2	1:D:240:SER:C	2.32	0.50
1:J:435:SER:OG	1:J:562:ARG:NH2	2.43	0.50
1:D:456:GLN:HA	1:D:477:ARG:HA	1.93	0.50
2:H:91:THR:HG22	2:H:119:VAL:N	2.26	0.50
3:I:8:PRO:HB2	3:I:11:LEU:CD1	2.41	0.50
1:J:447:ASP:CB	1:J:462:PRO:HG2	2.36	0.50
2:E:208:HIS:CD2	2:E:210:PRO:CG	2.95	0.50
1:G:545:GLN:HB3	1:G:546:PRO:HD3	1.93	0.50
3:I:7:SER:HB3	3:I:22:THR:HG1	1.76	0.50
1:J:338:MET:SD	1:J:401:PRO:HB3	2.52	0.50
3:L:142:PRO:HD2	3:L:199:HIS:HE1	1.76	0.50
1:A:367:THR:OG1	1:A:556:ASP:OD1	2.29	0.50
3:F:142:PRO:HD2	3:F:199:HIS:HE1	1.76	0.50
1:G:311:LEU:HD11	1:G:393:VAL:HG13	1.93	0.50
2:B:105:GLU:OE1	3:C:51:ARG:NE	2.45	0.49
2:B:132:LEU:HB2	2:B:147:GLY:HA3	1.93	0.49
3:C:8:PRO:HB2	3:C:11:LEU:CD1	2.42	0.49
1:A:435:SER:OG	1:A:562:ARG:NH2	2.44	0.49
3:C:142:PRO:HD2	3:C:199:HIS:HE1	1.76	0.49
3:I:142:PRO:HD2	3:I:199:HIS:HE1	1.76	0.49
1:J:466:ARG:NH1	1:J:466:ARG:CG	2.76	0.49
3:F:8:PRO:HB2	3:F:11:LEU:HD11	1.94	0.49
1:G:545:GLN:CB	1:G:546:PRO:CD	2.88	0.49



	to de pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:132:LEU:HB2	2:H:147:GLY:HA3	1.93	0.49
2:K:18:VAL:HG23	2:K:86:LEU:HD11	1.94	0.49
1:A:473:GLY:HA2	1:A:586:ARG:HG3	1.95	0.49
1:D:496:LYS:O	1:D:567:PRO:HA	2.12	0.49
1:G:191:PHE:CB	1:G:234:THR:HG23	2.42	0.49
3:I:141:TYR:HB3	3:I:142:PRO:HD3	1.94	0.49
1:A:447:ASP:CB	1:A:462:PRO:HG2	2.42	0.49
1:G:358:VAL:CG1	1:G:411:PRO:HB3	2.43	0.49
2:E:189:VAL:HG11	3:F:136:LEU:CD1	2.43	0.49
2:E:63:LYS:H	2:E:63:LYS:HG2	1.34	0.49
2:K:47:TRP:CD2	3:L:97:PRO:HG2	2.48	0.49
1:A:471:ARG:CA	1:A:507:ARG:NE	2.63	0.49
2:K:63:LYS:H	2:K:63:LYS:HG2	1.38	0.49
2:K:91:THR:HG22	2:K:119:VAL:N	2.26	0.49
2:K:132:LEU:HB2	2:K:147:GLY:HA3	1.94	0.48
1:J:191:PHE:HB2	1:J:234:THR:HG22	1.95	0.48
1:J:338:MET:CE	1:J:401:PRO:CB	2.67	0.48
2:H:105:GLU:OE1	3:I:51:ARG:NE	2.47	0.48
2:H:6:GLN:HA	2:H:21:SER:O	2.13	0.48
1:J:188:ILE:O	1:J:264:TYR:HA	2.14	0.48
3:C:141:TYR:HB3	3:C:142:PRO:HD3	1.95	0.48
2:E:132:LEU:HB2	2:E:147:GLY:HA3	1.94	0.48
1:J:301:ASP:OD1	1:J:303:ARG:HB2	2.13	0.48
1:A:291:GLU:OE1	1:A:334:ARG:NH2	2.47	0.48
3:F:18:ARG:O	3:I:7:SER:CB	2.61	0.48
1:D:188:ILE:O	1:D:264:TYR:HA	2.14	0.48
3:C:7:SER:HB3	3:C:22:THR:HG1	1.77	0.48
3:L:146:LYS:HA	3:L:146:LYS:HD3	1.57	0.48
3:F:141:TYR:HB3	3:F:142:PRO:HD3	1.96	0.48
2:B:6:GLN:HA	2:B:21:SER:O	2.14	0.47
3:C:82:GLU:H	3:C:82:GLU:HG3	1.42	0.47
3:C:62:ARG:HH12	3:C:80:GLN:CB	2.26	0.47
2:E:51:ILE:HD12	2:E:58:THR:HG22	1.96	0.47
3:I:146:LYS:HA	3:I:146:LYS:HD3	1.57	0.47
1:D:375:TYR:CE1	1:D:402:LEU:CD1	2.97	0.47
1:J:291:GLU:OE1	1:J:334:ARG:NH2	2.47	0.47
1:A:344:THR:O	1:A:387:ASN:ND2	2.47	0.47
1:A:352:THR:HG22	3:C:92:TYR:CD1	2.49	0.47
2:E:6:GLN:HA	2:E:21:SER:O	2.14	0.47
1:J:185:MET:CE	1:J:268:HIS:HD2	2.05	0.47
1:J:545:GLN:CD	1:J:546:PRO:HD3	2.35	0.47



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:188:ILE:O	1:A:264:TYR:HA	2.14	0.47
3:C:142:PRO:HD2	3:C:199:HIS:CE1	2.50	0.47
1:D:365:VAL:HG21	1:D:402:LEU:CD2	2.44	0.47
2:E:47:TRP:CD2	3:F:97:PRO:HG2	2.50	0.47
2:E:91:THR:HG22	2:E:119:VAL:N	2.26	0.47
3:F:142:PRO:HD2	3:F:199:HIS:CE1	2.49	0.47
3:F:146:LYS:HA	3:F:146:LYS:HD3	1.56	0.47
1:G:223:GLY:CA	1:G:469:SER:OG	2.62	0.47
2:H:62:PRO:HB2	3:L:96:PRO:HD3	1.96	0.47
2:H:189:VAL:CG1	3:I:136:LEU:HD11	2.43	0.47
3:I:3:GLN:NE2	3:L:3:GLN:OE1	2.47	0.47
1:J:453:SER:HB3	1:J:487:TRP:CE2	2.50	0.47
2:K:6:GLN:HA	2:K:21:SER:O	2.14	0.47
2:K:130:PHE:CE2	3:L:125:GLN:HG3	2.49	0.47
2:K:189:VAL:CG1	3:L:136:LEU:HD11	2.45	0.47
3:L:142:PRO:HD2	3:L:199:HIS:CE1	2.50	0.47
2:E:18:VAL:HG23	2:E:86:LEU:HD11	1.97	0.47
1:G:323:ASP:OD2	2:H:104:ARG:NH2	2.48	0.47
1:G:527:SER:HA	1:G:537:TYR:HA	1.97	0.47
1:J:480:GLN:HG2	1:J:578:TRP:HE1	1.79	0.47
1:A:445:ILE:O	1:A:445:ILE:HG22	2.14	0.47
1:A:531:ASN:HB3	1:A:533:LYS:CG	2.45	0.47
1:D:540:ASP:N	1:D:545:GLN:O	2.43	0.47
1:G:498:VAL:N	1:G:566:ILE:O	2.30	0.47
3:L:2:ILE:CD1	3:L:29:VAL:HG22	2.44	0.47
3:I:82:GLU:H	3:I:82:GLU:HG3	1.43	0.47
1:A:338:MET:HB3	1:A:338:MET:HE3	1.73	0.46
3:L:14:SER:O	3:L:17:ASP:HB2	2.15	0.46
3:C:8:PRO:HB2	3:C:11:LEU:HD11	1.96	0.46
3:C:146:LYS:HA	3:C:146:LYS:HD3	1.57	0.46
3:F:62:ARG:HH12	3:F:80:GLN:CB	2.28	0.46
1:G:452:ALA:HB2	1:G:474:TRP:HE1	1.79	0.46
1:J:460:TRP:CD1	1:J:460:TRP:O	2.69	0.46
1:A:447:ASP:CB	1:A:462:PRO:CG	2.93	0.46
1:D:291:GLU:OE1	1:D:334:ARG:NH2	2.48	0.46
1:D:539:GLN:HE22	1:D:546:PRO:HD3	1.79	0.46
3:C:30:SER:HB3	3:C:33:TYR:HD2	1.80	0.46
3:L:141:TYR:HB3	3:L:142:PRO:HD3	1.97	0.46
3:I:62:ARG:HH12	3:I:80:GLN:CB	2.28	0.46
2:B:43:LYS:HE3	3:C:86:THR:HG21	1.98	0.46
3:I:142:PRO:HD2	3:I:199:HIS:CE1	2.50	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:34:ILE:HD13	2:E:98:THR:HG22	1.98	0.46
2:H:18:VAL:HG23	2:H:86:LEU:HD11	1.97	0.46
3:L:24:THR:HA	3:L:70:THR:O	2.16	0.46
3:F:24:THR:HA	3:F:70:THR:O	2.16	0.46
1:G:427:CYS:HB2	1:G:431:ASP:OD2	2.16	0.46
3:I:2:ILE:CD1	3:I:29:VAL:HG22	2.46	0.46
3:L:30:SER:HB3	3:L:33:TYR:HD2	1.81	0.46
1:D:297:SER:OG	1:D:327:GLU:OE1	2.32	0.45
2:E:105:GLU:OE1	3:F:51:ARG:NE	2.49	0.45
3:I:30:SER:HB3	3:I:33:TYR:HD2	1.81	0.45
2:K:51:ILE:HD12	2:K:58:THR:HG22	1.99	0.45
1:D:427:CYS:HB2	1:D:431:ASP:OD2	2.15	0.45
2:E:199:THR:HB	2:E:200:LYS:HE3	1.98	0.45
1:J:375:TYR:CE1	1:J:402:LEU:HD12	2.48	0.45
3:L:48:LEU:HD23	3:L:59:VAL:HG21	1.98	0.45
3:L:62:ARG:HH12	3:L:80:GLN:CB	2.29	0.45
2:B:208:HIS:CD2	2:B:210:PRO:HG2	2.52	0.45
1:D:255:VAL:HG12	1:D:257:LYS:HE3	1.99	0.45
3:I:14:SER:O	3:I:17:ASP:HB2	2.16	0.45
2:B:18:VAL:HG23	2:B:86:LEU:HD11	1.96	0.45
3:F:30:SER:HB3	3:F:33:TYR:HD2	1.81	0.45
1:J:180:LEU:HD13	1:J:180:LEU:HA	1.81	0.45
1:A:478:ILE:HB	1:A:481:ALA:HB2	1.99	0.45
3:L:7:SER:HB3	3:L:22:THR:HG1	1.82	0.45
1:A:185:MET:HE3	1:A:268:HIS:HA	1.99	0.45
3:F:14:SER:O	3:F:17:ASP:HB2	2.17	0.45
1:A:545:GLN:HB3	1:A:546:PRO:HD2	1.98	0.45
3:C:24:THR:HA	3:C:70:THR:O	2.16	0.45
1:G:529:SER:HB2	1:G:535:TRP:HA	1.99	0.45
3:I:119:PHE:HE1	3:I:136:LEU:HD12	1.81	0.45
3:F:2:ILE:CD1	3:F:29:VAL:HG22	2.46	0.45
3:F:119:PHE:HE1	3:F:136:LEU:HD12	1.81	0.45
3:L:140:PHE:HB2	3:L:199:HIS:CE1	2.52	0.45
1:A:427:CYS:HB2	1:A:431:ASP:OD2	2.16	0.45
1:A:458:TYR:CD1	1:A:458:TYR:C	2.90	0.45
1:A:459:LEU:C	1:A:459:LEU:HD22	2.38	0.45
3:C:140:PHE:HB2	3:C:199:HIS:CE1	2.52	0.45
1:D:308:GLN:O	1:D:317:GLY:HA2	2.17	0.45
1:D:447:ASP:OD1	1:D:463:SER:N	2.49	0.45
2:E:189:VAL:HG13	3:F:136:LEU:HD11	1.99	0.45
1:G:211:ASP:OD1	1:G:252:ASP:N	2.49	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:208:HIS:CD2	2:H:210:PRO:CD	2.99	0.45
1:J:255:VAL:HG12	1:J:257:LYS:HE3	1.99	0.45
2:B:208:HIS:CD2	2:B:210:PRO:CD	3.00	0.44
3:I:24:THR:HA	3:I:70:THR:O	2.17	0.44
2:K:34:ILE:HD13	2:K:98:THR:HG22	1.99	0.44
1:A:341:ALA:HB3	1:A:425:PHE:HB2	1.99	0.44
2:B:34:ILE:HD13	2:B:98:THR:HG22	1.98	0.44
3:C:62:ARG:HH12	3:C:80:GLN:CG	2.30	0.44
3:F:140:PHE:HB2	3:F:199:HIS:CE1	2.52	0.44
1:G:255:VAL:HG12	1:G:257:LYS:HE3	1.98	0.44
1:J:181:ALA:HB2	1:J:266:LEU:CD2	2.45	0.44
3:C:2:ILE:CD1	3:C:29:VAL:HG22	2.48	0.44
2:E:30:LYS:HE2	2:E:74:THR:CG2	2.47	0.44
2:H:34:ILE:HD13	2:H:98:THR:HG22	1.98	0.44
1:J:375:TYR:HE1	1:J:402:LEU:HD12	1.82	0.44
1:J:427:CYS:HB2	1:J:431:ASP:OD2	2.17	0.44
2:K:208:HIS:CD2	2:K:210:PRO:HG2	2.51	0.44
1:D:375:TYR:CE1	1:D:402:LEU:HD13	2.52	0.44
2:E:208:HIS:CD2	2:E:210:PRO:CD	3.00	0.44
1:G:222:VAL:HG13	1:G:466:ARG:CZ	2.47	0.44
2:H:208:HIS:CD2	2:H:210:PRO:HG2	2.52	0.44
1:J:453:SER:HB3	1:J:487:TRP:CG	2.52	0.44
1:J:528:TYR:CE2	1:J:566:ILE:HG23	2.52	0.44
3:C:14:SER:O	3:C:17:ASP:HB2	2.17	0.44
1:D:181:ALA:HB2	1:D:266:LEU:CD2	2.44	0.44
2:E:208:HIS:CD2	2:E:210:PRO:HG2	2.52	0.44
1:G:223:GLY:CA	1:G:469:SER:HG	2.31	0.44
2:B:132:LEU:HB3	3:C:119:PHE:CD2	2.53	0.44
2:B:189:VAL:HG13	3:C:136:LEU:HD11	1.98	0.44
1:J:458:TYR:CD1	1:J:458:TYR:C	2.90	0.44
1:D:211:ASP:OD1	1:D:252:ASP:N	2.49	0.44
1:D:338:MET:SD	1:D:403:LEU:HD13	2.57	0.44
1:D:460:TRP:CD1	1:D:460:TRP:N	2.86	0.44
3:F:187:TYR:HA	3:F:193:TYR:OH	2.18	0.44
1:J:308:GLN:O	1:J:317:GLY:HA2	2.18	0.44
1:J:341:ALA:HB3	1:J:425:PHE:HB2	1.98	0.44
1:A:255:VAL:HG12	1:A:257:LYS:HE3	1.99	0.44
2:E:130:PHE:CE2	3:F:125:GLN:HG3	2.53	0.44
3:F:29:VAL:HG13	3:F:93:TYR:HB2	2.00	0.44
3:I:140:PHE:HB2	3:I:199:HIS:CE1	2.53	0.44
2:K:47:TRP:CG	3:L:97:PRO:HG2	2.53	0.44



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:208:HIS:CD2	2:K:210:PRO:CD	3.00	0.44
1:D:531:ASN:HB3	1:D:533:LYS:CG	2.48	0.43
1:A:447:ASP:HB3	1:A:462:PRO:HG2	2.01	0.43
2:B:63:LYS:H	2:B:63:LYS:HG2	1.35	0.43
1:D:341:ALA:HB3	1:D:425:PHE:HB2	1.99	0.43
1:D:459:LEU:HD22	1:D:459:LEU:C	2.39	0.43
1:G:308:GLN:O	1:G:317:GLY:HA2	2.18	0.43
2:H:199:THR:HB	2:H:200:LYS:HE3	1.99	0.43
1:J:449:GLN:HE21	1:J:449:GLN:HB3	1.57	0.43
1:J:538:ILE:CD1	1:J:566:ILE:HD13	2.48	0.43
1:D:472:SER:HB2	1:D:473:GLY:H	1.67	0.43
1:D:557:THR:HA	1:D:558:PRO:HD3	1.89	0.43
1:G:239:ARG:HH11	1:G:239:ARG:HG2	1.84	0.43
1:J:444:LEU:HD12	1:J:444:LEU:HA	1.89	0.43
3:L:119:PHE:HE1	3:L:136:LEU:HD12	1.82	0.43
3:L:187:TYR:HA	3:L:193:TYR:OH	2.19	0.43
1:A:308:GLN:O	1:A:317:GLY:HA2	2.17	0.43
1:A:460:TRP:O	1:A:460:TRP:CD1	2.71	0.43
1:J:211:ASP:OD1	1:J:252:ASP:N	2.48	0.43
3:C:119:PHE:HE1	3:C:136:LEU:HD12	1.82	0.43
1:G:363:LEU:HD23	1:G:375:TYR:CB	2.48	0.43
3:I:187:TYR:HA	3:I:193:TYR:OH	2.19	0.43
2:K:132:LEU:HB3	3:L:119:PHE:CD2	2.53	0.43
1:D:460:TRP:CD1	1:D:460:TRP:O	2.71	0.43
2:K:199:THR:HB	2:K:200:LYS:HE3	2.00	0.43
1:D:467:LEU:HA	1:D:586:ARG:HB3	2.00	0.43
3:C:80:GLN:HB3	3:C:81:PRO:HD2	2.00	0.43
1:D:443:GLY:HA2	1:D:466:ARG:HH12	1.82	0.43
3:F:18:ARG:O	3:I:7:SER:HB3	2.19	0.43
3:F:53:SER:CB	3:F:65:GLY:HA3	2.49	0.43
3:I:62:ARG:HH12	3:I:80:GLN:CG	2.32	0.43
1:A:471:ARG:CB	1:A:507:ARG:CZ	2.97	0.42
1:D:352:THR:HG22	3:F:92:TYR:CD1	2.54	0.42
2:E:132:LEU:HB3	3:F:119:PHE:CD2	2.53	0.42
3:F:80:GLN:HB3	3:F:81:PRO:HD2	2.01	0.42
1:G:402:LEU:HD23	1:G:402:LEU:HA	1.88	0.42
1:A:440:MET:O	1:A:466:ARG:HD2	2.19	0.42
1:A:471:ARG:HB3	1:A:507:ARG:NH2	2.35	0.42
3:I:3:GLN:OE1	3:L:3:GLN:NE2	2.52	0.42
2:B:164:SER:HB2	1:D:322:LEU:CD1	2.47	0.42
3:F:108:LYS:HA	3:F:141:TYR:OH	2.20	0.42



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:28:ASN:O	2:K:29:ILE:HB	2.19	0.42
3:L:108:LYS:HA	3:L:141:TYR:OH	2.19	0.42
3:C:53:SER:CB	3:C:65:GLY:HA3	2.49	0.42
3:F:7:SER:HB3	3:F:22:THR:HG1	1.84	0.42
1:G:229:TYR:CE2	1:G:235:PRO:HB3	2.54	0.42
1:J:338:MET:HE2	1:J:338:MET:HB3	1.72	0.42
3:L:82:GLU:H	3:L:82:GLU:HG3	1.43	0.42
3:C:187:TYR:HA	3:C:193:TYR:OH	2.20	0.42
1:G:438:LEU:HD12	1:G:589:VAL:HG12	2.01	0.42
1:G:452:ALA:HB1	1:G:474:TRP:HE1	1.83	0.42
1:G:523:LYS:HB3	1:G:548:LEU:HD11	2.00	0.42
1:J:374:VAL:HG11	1:J:381:HIS:ND1	2.35	0.42
1:J:447:ASP:HB3	1:J:462:PRO:CB	2.42	0.42
2:B:32:TYR:CD1	2:B:32:TYR:N	2.87	0.42
3:F:119:PHE:CE1	3:F:136:LEU:HD12	2.54	0.42
1:J:445:ILE:O	1:J:445:ILE:HG22	2.19	0.42
2:E:28:ASN:O	2:E:29:ILE:HB	2.20	0.42
1:G:437:MET:HE2	1:G:588:GLU:HG2	1.99	0.42
2:H:63:LYS:H	2:H:63:LYS:HG2	1.33	0.42
1:A:169:TYR:HE2	1:A:257:LYS:HB2	1.85	0.42
1:D:475:PHE:HA	1:D:476:PRO:HD3	1.91	0.42
3:F:2:ILE:HD11	3:F:29:VAL:CG2	2.50	0.42
1:G:351:GLU:HG3	3:I:93:TYR:O	2.20	0.42
3:I:80:GLN:HB3	3:I:81:PRO:HD2	2.01	0.42
3:I:119:PHE:CE1	3:I:136:LEU:HD12	2.54	0.42
1:J:169:TYR:HE2	1:J:257:LYS:HB2	1.85	0.42
1:A:455:THR:OG1	1:A:460:TRP:HB3	2.20	0.42
2:B:107:TRP:HA	3:C:35:HIS:CD2	2.55	0.42
2:B:189:VAL:CG1	3:C:136:LEU:HD11	2.50	0.42
2:H:18:VAL:O	2:H:82:GLU:HA	2.20	0.42
3:I:53:SER:CB	3:I:65:GLY:HA3	2.49	0.42
1:J:338:MET:SD	1:J:403:LEU:HD12	2.60	0.42
1:A:185:MET:HE3	1:A:268:HIS:CD2	2.50	0.41
1:A:540:ASP:HB2	1:A:547:LYS:HB2	2.02	0.41
3:C:108:LYS:HA	3:C:141:TYR:OH	2.20	0.41
1:D:169:TYR:HE2	1:D:257:LYS:HB2	1.85	0.41
2:E:137:ARG:H	2:E:137:ARG:HG2	1.63	0.41
1:G:239:ARG:HH11	1:G:239:ARG:CG	2.33	0.41
2:H:87:ARG:HG3	1:J:314:ASP:HB2	2.01	0.41
3:I:29:VAL:HG13	3:I:93:TYR:HB2	2.02	0.41
1:J:531:ASN:HB3	1:J:533:LYS:CG	2.49	0.41



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:L:53:SER:CB	3:L:65:GLY:HA3	2.50	0.41
2:B:189:VAL:CG1	3:C:136:LEU:CD1	2.97	0.41
1:D:376:ARG:HG2	1:D:381:HIS:HA	2.02	0.41
1:D:440:MET:O	1:D:466:ARG:NH1	2.50	0.41
1:G:451:SER:OG	1:G:489:GLN:HB3	2.21	0.41
2:H:32:TYR:CD1	2:H:32:TYR:N	2.87	0.41
3:L:137:LEU:N	3:L:137:LEU:CD2	2.80	0.41
1:A:405:ARG:HG2	1:A:406:PHE:CD2	2.55	0.41
2:B:47:TRP:CD2	3:C:97:PRO:HG2	2.56	0.41
1:G:174:ASP:OD1	1:G:250:HIS:ND1	2.34	0.41
1:J:456:GLN:N	1:J:475:PHE:O	2.41	0.41
1:J:567:PRO:HB2	1:J:594:TRP:HZ2	1.86	0.41
2:K:43:LYS:HE3	3:L:86:THR:CG2	2.49	0.41
3:L:53:SER:O	3:L:65:GLY:CA	2.68	0.41
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.90	0.41
2:B:84:SER:O	2:B:85:SER:C	2.59	0.41
2:B:199:THR:HB	2:B:200:LYS:HE3	2.02	0.41
3:F:137:LEU:N	3:F:137:LEU:CD2	2.80	0.41
1:G:373:MET:HG3	1:G:554:HIS:CG	2.55	0.41
2:K:18:VAL:HG23	2:K:86:LEU:HD21	2.03	0.41
2:E:189:VAL:CG1	3:F:136:LEU:CD1	2.99	0.41
1:G:314:ASP:HB2	2:K:87:ARG:HG3	2.01	0.41
1:G:362:LYS:HE2	1:G:381:HIS:HB3	2.03	0.41
2:K:135:CYS:HB2	3:L:215:CYS:HB3	2.02	0.41
3:C:29:VAL:HG13	3:C:93:TYR:HB2	2.03	0.41
2:E:32:TYR:CD1	2:E:32:TYR:N	2.86	0.41
1:G:447:ASP:HA	1:G:450:ILE:CD1	2.50	0.41
2:H:84:SER:O	2:H:85:SER:C	2.59	0.41
3:I:53:SER:O	3:I:65:GLY:CA	2.68	0.41
3:I:108:LYS:HA	3:I:141:TYR:OH	2.20	0.41
2:K:6:GLN:HE21	2:K:6:GLN:HB3	1.76	0.41
3:L:80:GLN:HB3	3:L:81:PRO:HD2	2.02	0.41
1:G:464:ALA:HA	1:G:470:SER:HB2	2.03	0.41
2:H:132:LEU:HB3	3:I:119:PHE:CD2	2.56	0.41
1:J:528:TYR:CE2	1:J:566:ILE:CG2	3.03	0.41
1:J:557:THR:HA	1:J:558:PRO:HD3	1.89	0.41
2:B:18:VAL:O	2:B:82:GLU:HA	2.21	0.41
3:C:119:PHE:CE1	3:C:136:LEU:HD12	2.55	0.41
3:F:53:SER:O	3:F:65:GLY:CA	2.68	0.41
1:G:169:TYR:HE2	1:G:257:LYS:HB2	1.85	0.41
2:K:137:ARG:H	2:K:137:ARG:HG2	1.62	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:191:PHE:HB2	1:A:234:THR:HG22	2.01	0.41
1:A:371:ASP:HB3	1:A:555:TYR:OH	2.21	0.41
1:A:496:LYS:O	1:A:567:PRO:HA	2.21	0.41
1:A:499:LYS:HG3	1:A:565:PRO:HB3	2.02	0.41
2:B:6:GLN:HE21	2:B:6:GLN:HB3	1.75	0.41
2:B:30:LYS:HD2	2:B:54:GLU:HG3	2.03	0.41
1:G:474:TRP:O	1:G:474:TRP:CE3	2.74	0.41
1:G:497:THR:HA	1:G:567:PRO:HA	2.02	0.41
3:I:2:ILE:HD11	3:I:29:VAL:CG2	2.51	0.41
1:J:496:LYS:O	1:J:567:PRO:HA	2.21	0.41
2:K:87:ARG:HB3	2:K:89:GLU:HG2	2.03	0.41
3:L:119:PHE:CE1	3:L:136:LEU:HD12	2.55	0.41
1:A:345:GLN:HA	1:A:387:ASN:ND2	2.36	0.41
1:A:456:GLN:CA	1:A:477:ARG:HA	2.50	0.41
3:C:6:GLN:HG3	3:C:100:GLY:HA3	2.03	0.41
3:C:201:GLY:O	3:C:202:LEU:HG	2.21	0.41
1:D:173:LEU:HB2	1:D:251:THR:OG1	2.21	0.41
1:A:184:LYS:HE3	1:A:268:HIS:CE1	2.55	0.40
3:C:53:SER:O	3:C:65:GLY:CA	2.69	0.40
2:H:18:VAL:HG23	2:H:86:LEU:HD21	2.03	0.40
3:I:6:GLN:HE21	3:I:100:GLY:HA3	1.86	0.40
3:L:2:ILE:HD11	3:L:29:VAL:CG2	2.49	0.40
1:G:198:HIS:CE1	1:G:255:VAL:HB	2.56	0.40
1:A:438:LEU:HD12	1:A:589:VAL:HG12	2.04	0.40
1:G:173:LEU:HB2	1:G:251:THR:OG1	2.22	0.40
1:G:453:SER:OG	1:G:486:GLU:OE1	2.30	0.40
1:G:529:SER:O	1:G:568:ALA:HB1	2.21	0.40
1:G:545:GLN:CB	1:G:546:PRO:HD2	2.47	0.40
3:I:37:TYR:HE2	3:I:90:HIS:HB3	1.86	0.40
1:J:180:LEU:HD13	1:J:243:GLY:O	2.21	0.40
1:J:438:LEU:HD12	1:J:589:VAL:HG12	2.02	0.40
1:G:224:PRO:HD3	1:G:469:SER:OG	2.21	0.40
1:J:463:SER:CA	1:J:466:ARG:HD2	2.49	0.40
1:J:540:ASP:OD1	1:J:542:ARG:HD3	2.21	0.40
2:K:18:VAL:O	2:K:82:GLU:HA	2.21	0.40
2:K:32:TYR:CD1	2:K:32:TYR:N	2.87	0.40
3:L:37:TYR:HE2	3:L:90:HIS:HB3	1.86	0.40
1:A:217:ASP:HB3	1:A:224:PRO:HG2	2.03	0.40
3:F:37:TYR:HE2	3:F:90:HIS:HB3	1.86	0.40
3:I:137:LEU:HD13	3:I:197:VAL:CG1	2.51	0.40
1:J:301:ASP:OD1	1:J:303:ARG:CB	2.70	0.40



All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:PHE:O	$1:G:531:ASN:OD1[2_546]$	1.96	0.24

## 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	entiles
1	А	418/583~(72%)	393 (94%)	23~(6%)	2~(0%)	29	67
1	D	412/583~(71%)	390~(95%)	20~(5%)	2~(0%)	29	67
1	G	388/583~(67%)	365 (94%)	18 (5%)	5 (1%)	12	47
1	J	419/583~(72%)	391 (93%)	23~(6%)	5 (1%)	13	49
2	В	217/228~(95%)	199 (92%)	16 (7%)	2(1%)	17	56
2	Ε	218/228~(96%)	200 (92%)	16 (7%)	2(1%)	17	56
2	Η	218/228~(96%)	200 (92%)	16 (7%)	2(1%)	17	56
2	Κ	218/228~(96%)	201 (92%)	15 (7%)	2(1%)	17	56
3	С	213/215~(99%)	204 (96%)	9 (4%)	0	100	100
3	F	213/215~(99%)	204 (96%)	9~(4%)	0	100	100
3	Ι	213/215~(99%)	204 (96%)	9 (4%)	0	100	100
3	L	213/215~(99%)	204 (96%)	9 (4%)	0	100	100
All	All	3360/4104~(82%)	3155 (94%)	183 (5%)	22 (1%)	22	61

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	29	ILE
2	В	43	LYS
2	Е	29	ILE
1	G	545	GLN



Mol	Chain	Res	Type
2	Н	29	ILE
2	Н	43	LYS
1	J	545	GLN
2	Κ	29	ILE
2	Κ	43	LYS
2	Е	43	LYS
1	G	375	TYR
1	G	466	ARG
1	G	544	GLN
1	J	472	SER
1	А	273	GLU
1	D	546	PRO
1	J	457	GLU
1	J	479	PRO
1	А	255	VAL
1	D	255	VAL
1	G	255	VAL
1	J	255	VAL

#### 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	Percentiles
1	А	372/506~(74%)	331 (89%)	41 (11%)	6 26
1	D	363/506~(72%)	323~(89%)	40 (11%)	6 26
1	G	350/506~(69%)	313~(89%)	37~(11%)	6 27
1	J	372/506~(74%)	324 (87%)	48 (13%)	4 19
2	В	187/194~(96%)	145 (78%)	42 (22%)	1 4
2	Е	187/194~(96%)	144 (77%)	43 (23%)	1 3
2	Н	187/194~(96%)	146 (78%)	41 (22%)	1 5
2	Κ	187/194~(96%)	146 (78%)	41 (22%)	1 5
3	С	190/190~(100%)	142 (75%)	48 (25%)	0 2
3	F	190/190~(100%)	145 (76%)	45 (24%)	1 3



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	Ι	190/190~(100%)	142~(75%)	48 (25%)	0 2
3	L	190/190~(100%)	143~(75%)	47 (25%)	0 2
All	All	2965/3560~(83%)	2444 (82%)	521 (18%)	2 9

All (521) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	155	SER
1	А	161	GLU
1	А	167	GLU
1	А	175	CYS
1	А	185	MET
1	А	209	LYS
1	А	210	TYR
1	А	233	LYS
1	А	239	ARG
1	А	248	THR
1	А	252	ASP
1	А	270	GLU
1	А	300	SER
1	А	322	LEU
1	А	350	ARG
1	А	370	GLU
1	А	373	MET
1	А	379	LYS
1	А	387	ASN
1	А	391	THR
1	А	392	GLU
1	А	397	LYS
1	А	399	HIS
1	А	410	ARG
1	А	444	LEU
1	А	447	ASP
1	А	448	SER
1	А	450	ILE
1	А	454	SER
1	А	455	THR
1	А	458	TYR
1	А	459	LEU
1	А	460	TRP
1	А	467	LEU



Mol	Chain	Res	Type
1	А	469	SER
1	А	471	ARG
1	А	518	ARG
1	А	542	ARG
1	А	543	THR
1	А	566	ILE
1	А	577	ARG
2	В	1	GLU
2	В	12	LYS
2	В	20	ILE
2	В	21	SER
2	В	30	LYS
2	В	32	TYR
2	В	33	TYR
2	В	39	GLN
2	В	43	LYS
2	В	50	ARG
2	В	55	ASP
2	В	56	ASP
2	В	59	LYS
2	В	63	LYS
2	В	65	GLN
2	В	69	THR
2	В	70	ILE
2	В	71	THR
2	В	74	THR
2	В	83	LEU
2	В	84	SER
2	В	88	SER
2	B	100	ILE
2	В	104	ARG
2	В	105	GLU
2	В	116	LEU
2	В	123	SER
2	B	125	LYS
2	В	137	ARG
2	В	138	SER
2	В	139	THR
2	В	141	GLU
2	В	151	LYS
2	В	169	SER
2	В	177	VAL



Mol	Chain	Res	Type
2	В	178	LEU
2	В	187	SER
2	В	189	VAL
2	В	195	SER
2	В	197	LEU
2	В	199	THR
2	В	200	LYS
3	С	2	ILE
3	С	3	GLN
3	С	10	SER
3	С	14	SER
3	С	18	ARG
3	С	19	VAL
3	С	24	THR
3	С	32	SER
3	С	34	LEU
3	С	43	LYS
3	С	49	ILE
3	С	52	THR
3	С	53	SER
3	С	59	VAL
3	С	62	ARG
3	С	64	SER
3	С	73	THR
3	С	78	SER
3	С	82	GLU
3	С	92	TYR
3	С	94	ARG
3	C	95	SER
3	С	98	THR
3	C	104	LYS
3	C	106	GLU
3	С	115	SER
3	C	118	ILE
3	С	122	SER
3	С	130	THR
3	С	132	SER
3	С	137	LEU
3	С	143	ARG
3	С	146	LYS
3	С	147	VAL
3	С	155	LEU



Mol	Chain	Res	Type
3	С	157	SER
3	С	169	SER
3	С	171	ASP
3	С	172	SER
3	С	177	SER
3	С	180	LEU
3	С	181	THR
3	С	186	ASP
3	С	191	LYS
3	С	198	THR
3	С	204	SER
3	С	208	LYS
3	С	214	GLU
1	D	149	CYS
1	D	155	SER
1	D	161	GLU
1	D	167	GLU
1	D	175	CYS
1	D	185	MET
1	D	209	LYS
1	D	210	TYR
1	D	233	LYS
1	D	234	THR
1	D	241	SER
1	D	248	THR
1	D	252	ASP
1	D	322	LEU
1	D	350	ARG
1	D	379	LYS
1	D	385	GLN
1	D	397	LYS
1	D	402	LEU
1	D	403	LEU
1	D	444	LEU
1	D	447	ASP
1	D	448	SER
1	D	450	ILE
1	D	451	SER
1	D	454	SER
1	D	457	GLU
1	D	458	TYR
1	D	459	LEU



Mol	Chain	Res	Type
1	D	460	TRP
1	D	463	SER
1	D	466	ARG
1	D	467	LEU
1	D	469	SER
1	D	472	SER
1	D	494	THR
1	D	518	ARG
1	D	544	GLN
1	D	566	ILE
1	D	577	ARG
2	Е	1	GLU
2	Е	12	LYS
2	Е	20	ILE
2	Е	21	SER
2	Е	32	TYR
2	Е	33	TYR
2	Е	39	GLN
2	Е	43	LYS
2	Е	50	ARG
2	Е	54	GLU
2	Е	55	ASP
2	Е	56	ASP
2	Е	59	LYS
2	Е	63	LYS
2	Е	65	GLN
2	Е	69	THR
2	Е	70	ILE
2	Е	71	THR
2	E	74	THR
2	Е	83	LEU
2	E	84	SER
2	Е	88	SER
2	E	100	ILE
2	Е	104	ARG
2	E	105	GLU
2	E	116	LEU
2	E	123	SER
2	E	125	LYS
2	E	137	ARG
2	E	138	SER
2	E	139	THR



Mol	Chain	Res	Type
2	Е	141	GLU
2	Е	151	LYS
2	Е	168	THR
2	Е	169	SER
2	Е	177	VAL
2	Е	178	LEU
2	Е	187	SER
2	Е	189	VAL
2	Е	195	SER
2	Е	197	LEU
2	Е	199	THR
2	Е	200	LYS
3	F	3	GLN
3	F	10	SER
3	F	14	SER
3	F	18	ARG
3	F	19	VAL
3	F	24	THR
3	F	32	SER
3	F	34	LEU
3	F	43	LYS
3	F	49	ILE
3	F	52	THR
3	F	53	SER
3	F	59	VAL
3	F	62	ARG
3	F	64	SER
3	F	73	THR
3	F	78	SER
3	F	82	GLU
3	F	92	TYR
3	F	94	ARG
3	F	95	SER
3	F	98	THR
3	F	106	GLU
3	F	118	ILE
3	F	122	SER
3	F	130	THR
3	F	132	SER
3	F	137	LEU
3	F	143	ARG
3	F	146	LYS



Mol	Chain	Res	Type
3	F	147	VAL
3	F	155	LEU
3	F	157	SER
3	F	169	SER
3	F	171	ASP
3	F	172	SER
3	F	177	SER
3	F	180	LEU
3	F	181	THR
3	F	186	ASP
3	F	191	LYS
3	F	198	THR
3	F	204	SER
3	F	208	LYS
3	F	214	GLU
1	G	155	SER
1	G	161	GLU
1	G	167	GLU
1	G	175	CYS
1	G	209	LYS
1	G	210	TYR
1	G	233	LYS
1	G	239	ARG
1	G	248	THR
1	G	252	ASP
1	G	269	GLN
1	G	298	THR
1	G	300	SER
1	G	322	LEU
1	G	336	LEU
1	G	350	ARG
1	G	371	ASP
1	G	383	VAL
1	G	398	LEU
1	G	402	LEU
1	G	403	LEU
1	G	444	LEU
1	G	461	SER
1	G	463	SER
1	G	467	LEU
1	G	469	SER
1	G	474	TRP



Mol	Chain	Res	Type
1	G	533	LYS
1	G	534	ASP
1	G	540	ASP
1	G	542	ARG
1	G	544	GLN
1	G	555	TYR
1	G	564	ASP
1	G	566	ILE
1	G	569	GLN
1	G	577	ARG
2	Н	1	GLU
2	Н	12	LYS
2	Н	20	ILE
2	Н	21	SER
2	Н	32	TYR
2	Н	33	TYR
2	Н	39	GLN
2	Н	43	LYS
2	Н	50	ARG
2	Н	54	GLU
2	Н	55	ASP
2	Н	56	ASP
2	Н	59	LYS
2	Н	63	LYS
2	Н	65	GLN
2	Н	69	THR
2	Н	70	ILE
2	Н	71	THR
2	Н	74	THR
2	Н	83	LEU
2	Н	84	SER
2	Н	88	SER
2	Н	100	ILE
2	Н	104	ARG
2	Н	116	LEU
2	H	123	SER
2	Н	125	LYS
2	Η	137	ARG
2	Н	138	SER
2	Н	139	THR
2	Н	141	GLU
2	Н	151	LYS



Mol	Chain	Res	Type
2	Н	169	SER
$\frac{2}{2}$	H	177	VAL
2	H	178	LEU
2	H	187	SEB
2	H	189	VAL
2	H	195	SER
2	H	197	LEU
2	H	199	THR
2	H	200	LYS
3	I	2	ILE
3	I	3	GLN
3	I	10	SER
3	I	14	SER
3	Ī	18	ARG
3	I	19	VAL
3	Ι	24	THR
3	Ι	32	SER
3	Ι	34	LEU
3	Ι	43	LYS
3	Ι	49	ILE
3	Ι	52	THR
3	Ι	53	SER
3	Ι	59	VAL
3	Ι	62	ARG
3	Ι	64	SER
3	Ι	73	THR
3	Ι	78	SER
3	Ι	82	GLU
3	Ι	92	TYR
3	Ι	94	ARG
3	Ι	95	SER
3	Ι	98	THR
3	Ι	104	LYS
3	Ι	106	GLU
3	Ι	115	SER
3	Ι	118	ILE
3	Ι	122	SER
3	Ι	130	THR
3	Ι	132	SER
3	Ι	137	LEU
3	Ι	143	ARG
3	Ι	146	LYS



Mol	Chain	Res	Type
3	Ι	147	VAL
3	Ι	155	LEU
3	Ι	157	SER
3	Ι	169	SER
3	Ι	171	ASP
3	Ι	172	SER
3	Ι	177	SER
3	Ι	180	LEU
3	Ι	181	THR
3	Ι	186	ASP
3	Ι	191	LYS
3	Ι	198	THR
3	Ι	204	SER
3	Ι	208	LYS
3	Ι	214	GLU
1	J	151	LYS
1	J	155	SER
1	J	161	GLU
1	J	167	GLU
1	J	175	CYS
1	J	180	LEU
1	J	185	MET
1	J	209	LYS
1	J	210	TYR
1	J	233	LYS
1	J	248	THR
1	J	252	ASP
1	J	269	GLN
1	J	300	SER
1	J	322	LEU
1	J	350	ARG
1	J	353	GLN
1	J	379	LYS
1	J	383	VAL
1	J	399	HIS
1	J	401	PRO
1	J	402	LEU
1	J	444	LEU
1	J	447	ASP
1	J	449	GLN
1	J	450	ILE
1	J	454	SER



Mol	Chain	Res	Type
1	J	455	THR
1	J	458	TYR
1	J	459	LEU
1	J	460	TRP
1	J	463	SER
1	J	466	ARG
1	J	469	SER
1	J	471	ARG
1	J	475	PHE
1	J	477	ARG
1	J	478	ILE
1	J	480	GLN
1	J	482	GLN
1	J	494	THR
1	J	518	ARG
1	J	539	GLN
1	J	542	ARG
1	J	543	THR
1	J	544	GLN
1	J	545	GLN
1	J	566	ILE
2	Κ	1	GLU
2	Κ	12	LYS
2	Κ	20	ILE
2	Κ	21	SER
2	Κ	32	TYR
2	Κ	33	TYR
2	Κ	39	GLN
2	K	43	LYS
2	K	50	ARG
2	K	54	GLU
2	K	55	ASP
2	K	56	ASP
2	K	59	LYS
2	K	63	LYS
2	K	65	GLN
2	K	69	THR
2	K	70	ILE
2	K	71	THR
2	K	74	THR
2	K	83	LEU
2	K	84	SER



Mol	Chain	Res	Type
2	K	88	SER
2	K	100	ILE
2	K	104	ARG
2	К	105	GLU
2	K	116	LEU
2	K	123	SER
2	K	125	LYS
2	K	137	ARG
2	K	138	SER
2	K	139	THR
2	K	141	GLU
2	K	151	LYS
2	K	177	VAL
2	K	178	LEU
2	K	187	SER
2	K	189	VAL
2	K	195	SER
2	K	197	LEU
2	K	199	THR
2	К	200	LYS
3	L	2	ILE
3	L	3	GLN
3	L	10	SER
3	L	14	SER
3	L	18	ARG
3	L	19	VAL
3	L	24	THR
3	L	32	SER
3	L	34	LEU
3	L	43	LYS
3	L	49	ILE
3	L	52	THR
3	L	53	SER
3	L	59	VAL
3	L	62	ARG
3	L	64	SER
3	L	73	THR
3	L	78	SER
3	L	82	GLU
3	L	92	TYR
3	L	94	ARG
3	L	95	SER



Mol	Chain	Res	Type
2	T	08	ТИР
<u> </u>		90	
3	L	106	GLU
3	L	115	SER
3	L	118	ILE
3	L	122	SER
3	L	130	THR
3	L	132	SER
3	L	137	LEU
3	L	143	ARG
3	L	146	LYS
3	L	147	VAL
3	L	155	LEU
3	L	157	SER
3	L	169	SER
3	L	171	ASP
3	L	172	SER
3	L	177	SER
3	L	180	LEU
3	L	181	THR
3	L	186	ASP
3	L	191	LYS
3	L	198	THR
3	L	204	SER
3	L	208	LYS
3	L	214	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	268	HIS
1	А	353	GLN
1	А	387	ASN
1	А	531	ASN
2	В	3	GLN
2	В	39	GLN
3	С	3	GLN
3	С	6	GLN
3	С	159	ASN
1	D	190	GLN
1	D	353	GLN
1	D	380	ASN
1	D	381	HIS



Mol	Chain	Res	Type
1	D	531	ASN
1	D	544	GLN
1	D	569	GLN
2	Е	3	GLN
2	Е	39	GLN
3	F	3	GLN
3	F	6	GLN
3	F	159	ASN
1	G	353	GLN
1	G	377	HIS
1	G	388	ASN
1	G	399	HIS
1	G	449	GLN
1	G	544	GLN
1	G	545	GLN
2	Н	3	GLN
2	Н	39	GLN
3	Ι	3	GLN
3	Ι	6	GLN
3	Ι	159	ASN
1	J	268	HIS
1	J	377	HIS
1	J	380	ASN
1	J	531	ASN
1	J	539	GLN
1	J	545	GLN
1	J	569	GLN
2	K	3	GLN
2	K	39	GLN
3	L	3	GLN
3	L	6	GLN
3	L	159	ASN

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#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 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,  $95^{th}$  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	<rsrz></rsrz>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	426/583~(73%)	0.49	37 (8%) 10 5	37, 79, 167, 239	0
1	D	420/583~(72%)	0.59	55 (13%) 3 2	39, 110, 168, 220	0
1	G	402/583~(68%)	1.05	80 (19%) 1 1	42, 114, 196, 269	0
1	J	427/583~(73%)	0.77	70 (16%) 1 1	38, 111, 174, 256	0
2	В	219/228~(96%)	0.20	10 (4%) 32 20	35, 72, 122, 168	0
2	Е	220/228~(96%)	0.19	4 (1%) 68 55	36, 74, 131, 198	0
2	Н	220/228~(96%)	0.26	10 (4%) 33 21	34, 67, 124, 166	0
2	K	220/228~(96%)	0.21	5 (2%) 60 47	34, 70, 124, 161	0
3	С	215/215~(100%)	0.42	15 (6%) 16 9	28, 61, 135, 169	0
3	F	215/215~(100%)	0.43	18 (8%) 11 6	29, 62, 140, 159	0
3	Ι	215/215~(100%)	0.27	10 (4%) 31 19	29, 57, 122, 158	0
3	L	215/215~(100%)	0.37	16 (7%) 14 8	28, 65, 132, 152	0
All	All	3414/4104 (83%)	0.50	330 (9%) 7 4	28, 82, 160, 269	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	170	PRO	19.8
1	А	272	LEU	14.9
1	G	172	ASN	13.4
1	J	169	TYR	11.0
1	G	169	TYR	10.1
1	G	163	PRO	9.9
1	J	198	HIS	9.4
1	G	168	LYS	9.1
1	G	252	ASP	8.9
1	G	176	THR	8.6
1	G	170	PRO	8.1



8IV	W
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Mol	Chain	Res	Type	RSRZ
1	G	474	TRP	7.2
1	G	214	ASP	7.1
1	J	211	ASP	6.9
1	D	538	ILE	6.7
1	J	214	ASP	6.6
1	G	573	VAL	6.1
1	G	150	SER	6.0
1	А	163	PRO	5.9
1	G	210	TYR	5.9
1	J	212	TRP	5.7
1	G	211	ASP	5.6
2	Н	197	LEU	5.5
1	D	521	VAL	5.4
1	J	578	TRP	5.3
1	G	151	LYS	5.1
1	G	175	CYS	5.1
1	G	177	PHE	5.0
3	F	150	LYS	5.0
1	G	198	HIS	5.0
1	D	541	PRO	4.9
1	J	249	PHE	4.8
1	G	167	GLU	4.8
2	Н	138	SER	4.8
1	А	271	PRO	4.8
2	В	196	SER	4.7
3	Ι	211	ASN	4.7
2	Κ	28	ASN	4.7
1	G	583	ILE	4.7
1	D	226	ILE	4.6
1	J	475	PHE	4.6
1	G	248	THR	4.6
1	А	229	TYR	4.6
1	D	198	HIS	4.5
1	G	249	PHE	4.5
1	J	585	MET	4.4
1	А	273	GLU	4.3
1	D	211	ASP	4.3
1	J	256	ALA	4.2
1	А	544	GLN	4.1
1	J	213	LEU	4.1
1	G	253	MET	4.0
1	J	458	TYR	4.0



Mol	Chain	Res	Type	RSRZ
1	А	231	GLY	4.0
1	D	584	GLY	4.0
2	В	200	LYS	4.0
1	D	519	ALA	4.0
1	J	173	LEU	4.0
1	А	254	ALA	4.0
1	G	251	THR	4.0
1	А	172	ASN	4.0
1	D	227	GLY	3.9
1	J	272	LEU	3.9
2	В	197	LEU	3.9
1	D	172	ASN	3.9
3	L	179	THR	3.9
1	D	213	LEU	3.8
1	J	257	LYS	3.8
1	D	554	HIS	3.8
1	J	583	ILE	3.8
2	Н	200	LYS	3.7
1	G	219	ILE	3.7
1	J	474	TRP	3.7
1	G	216	TRP	3.7
1	D	196	LEU	3.7
2	Н	137	ARG	3.7
1	G	164	GLY	3.7
1	D	542	ARG	3.7
1	G	435	SER	3.7
1	G	173	LEU	3.6
1	G	578	TRP	3.6
3	Ι	130	THR	3.6
3	L	193	TYR	3.6
2	Н	201	THR	3.6
3	L	181	THR	3.6
1	J	227	GLY	3.5
1	G	229	TYR	3.5
1	J	228	LYS	3.5
1	D	585	MET	3.5
1	G	227	GLY	3.5
1	G	247	LEU	3.5
1	D	212	TRP	3.4
1	J	248	THR	3.4
1	J	546	PRO	3.4
1	А	251	THR	3.4



8IVW	
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Mol	Chain	Res	Type	RSRZ
1	G	574	TYR	3.4
1	G	213	LEU	3.4
3	С	182	LEU	3.4
3	F	180	LEU	3.4
3	С	187	TYR	3.4
1	G	378	GLY	3.4
1	G	166	PRO	3.4
1	D	552	ASN	3.4
1	G	476	PRO	3.3
1	J	525	LYS	3.3
1	D	528	TYR	3.3
1	G	565	PRO	3.3
1	J	524	PHE	3.3
1	J	258	ASP	3.3
3	L	136	LEU	3.3
1	J	226	ILE	3.2
1	G	270	GLU	3.2
1	G	149	CYS	3.2
1	D	570	TYR	3.2
2	Н	24	VAL	3.2
3	С	188	GLU	3.2
3	L	149	TRP	3.2
1	А	507	ARG	3.2
1	А	479	PRO	3.1
1	G	481	ALA	3.1
3	L	194	ALA	3.1
1	G	250	HIS	3.1
1	G	488	LEU	3.1
2	Е	137	ARG	3.1
3	F	53	SER	3.1
1	А	250	HIS	3.1
1	G	491	ASP	3.0
3	L	182	LEU	3.0
1	G	475	PHE	3.0
1	J	575	PRO	3.0
3	L	151	VAL	3.0
3	F	149	TRP	3.0
1	J	230	CYS	3.0
1	D	553	MET	3.0
1	D	249	PHE	3.0
3	С	184	LYS	2.9
3	Ι	209	SER	2.9



Mol	Chain	Res	Type	RSRZ
1	G	160	ILE	2.9
1	G	165	PHE	2.9
1	J	584	GLY	2.9
1	J	271	PRO	2.9
1	J	471	ARG	2.9
1	А	270	GLU	2.9
1	J	535	TRP	2.9
1	А	498	VAL	2.9
1	D	374	VAL	2.9
1	D	248	THR	2.9
3	F	187	TYR	2.9
1	А	226	ILE	2.9
1	А	499	LYS	2.9
1	А	428	ARG	2.9
1	G	262	ALA	2.9
3	С	159	ASN	2.8
1	J	148	ASP	2.8
1	J	486	GLU	2.8
1	D	169	TYR	2.8
1	J	506	ALA	2.8
1	J	488	LEU	2.8
1	А	429	VAL	2.8
1	А	211	ASP	2.8
1	J	473	GLY	2.8
1	G	524	PHE	2.8
3	С	210	PHE	2.8
3	L	138	ASN	2.8
1	G	499	LYS	2.8
1	А	227	GLY	2.8
1	G	551	GLY	2.8
1	A	215	ILE	2.8
1	J	532	GLY	2.8
1	А	506	ALA	2.7
3	С	193	TYR	2.7
1	J	450	ILE	2.7
3	L	180	LEU	2.7
1	G	212	TRP	2.7
3	Ι	140	PHE	2.7
1	J	171	HIS	2.7
2	Н	77	ASP	2.7
1	G	584	GLY	2.7
3	F	7	SER	2.7



Mol	Chain	Res	Type	RSRZ
1	J	537	TYR	2.7
2	В	137	ARG	2.7
3	С	214	GLU	2.7
3	Ι	193	TYR	2.7
1	J	266	LEU	2.7
2	В	131	PRO	2.7
2	В	185	SER	2.7
3	С	53	SER	2.7
3	F	138	ASN	2.7
1	J	194	PHE	2.6
3	Ι	210	PHE	2.6
1	G	498	VAL	2.6
1	G	590	LEU	2.6
3	С	121	PRO	2.6
3	F	136	LEU	2.6
1	D	247	LEU	2.6
3	С	52	THR	2.6
1	G	490	VAL	2.6
3	Ι	208	LYS	2.6
1	D	255	VAL	2.6
1	G	478	ILE	2.6
1	А	275	PHE	2.6
1	G	255	VAL	2.6
1	D	534	ASP	2.6
1	G	497	THR	2.6
1	J	215	ILE	2.6
1	D	246	SER	2.5
1	J	429	VAL	2.5
1	G	567	PRO	2.5
1	А	252	ASP	2.5
1	D	173	LEU	2.5
1	А	478	ILE	2.5
1	G	525	LYS	2.5
1	D	583	ILE	2.5
2	Κ	32	TYR	2.5
1	G	281	LEU	2.5
2	Κ	165	GLY	2.5
1	D	257	LYS	2.5
1	G	529	SER	2.5
1	J	503	ILE	2.5
1	J	225	LEU	2.5
1	J	526	VAL	2.5



8IV	VW
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Mol	Chain	Res	Type	RSRZ
3	Ι	199	HIS	2.5
3	L	209	SER	2.5
1	J	216	TRP	2.4
1	А	210	TYR	2.4
3	L	153	ASN	2.4
1	D	438	LEU	2.4
1	D	460	TRP	2.4
1	А	248	THR	2.4
1	G	520	PHE	2.4
1	J	255	VAL	2.4
1	J	229	TYR	2.4
1	А	214	ASP	2.4
1	J	573	VAL	2.4
2	Н	98	THR	2.4
3	F	153	ASN	2.4
1	J	576	GLU	2.4
1	G	225	LEU	2.4
3	Ι	138	ASN	2.4
1	G	228	LYS	2.4
1	G	162	SER	2.4
1	А	169	TYR	2.4
2	В	201	THR	2.4
1	G	585	MET	2.3
1	А	266	LEU	2.3
1	J	577	ARG	2.3
1	А	265	TYR	2.3
1	G	473	GLY	2.3
1	J	582	GLY	2.3
3	С	211	ASN	2.3
1	А	160	ILE	2.3
1	D	537	TYR	2.3
2	В	199	THR	2.3
3	F	197	VAL	2.3
1	D	576	GLU	2.3
1	G	263	ARG	2.3
2	Е	197	LEU	2.3
1	D	520	PHE	2.3
1	А	542	ARG	2.3
1	J	586	ARG	2.3
3	L	175	SER	2.3
1	G	519	ALA	2.3
1	J	519	ALA	2.3



8IVW	
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Mol	Chain	Res	Type	RSRZ
1	J	172	ASN	2.3
1	J	242	THR	2.3
3	F	118	ILE	2.3
1	А	171	HIS	2.3
1	D	498	VAL	2.3
2	Н	145	ALA	2.3
1	D	355	GLY	2.3
2	К	181	SER	2.3
3	Ι	7	SER	2.3
1	D	531	ASN	2.2
1	D	526	VAL	2.2
1	А	253	MET	2.2
1	G	178	THR	2.2
1	G	579	SER	2.2
1	G	257	LYS	2.2
2	Н	130	PHE	2.2
1	D	556	ASP	2.2
1	D	251	THR	2.2
1	D	522	ARG	2.2
3	С	7	SER	2.2
3	F	147	VAL	2.2
1	G	265	TYR	2.2
2	Е	172	HIS	2.2
1	D	175	CYS	2.2
1	А	474	TRP	2.2
3	F	193	TYR	2.2
1	D	591	GLY	2.2
1	G	153	PHE	2.2
1	D	573	VAL	2.2
1	D	587	LEU	2.1
3	L	210	PHE	2.1
3	L	118	ILE	2.1
3	F	139	ASN	2.1
1	D	256	ALA	2.1
1	J	191	PHE	2.1
2	В	198	GLY	2.1
1	D	467	LEU	2.1
3	С	179	THR	2.1
2	В	125	LYS	2.1
1	G	492	LEU	2.1
3	F	140	PHE	2.1
2	K	219	VAL	2.1



Mol	Chain	Res	Type	RSRZ
1	J	253	MET	2.1
1	D	177	PHE	2.1
2	Е	182	GLY	2.1
1	D	502	ILE	2.1
1	G	230	CYS	2.1
1	J	251	THR	2.1
1	J	156	PRO	2.1
3	С	122	SER	2.1
3	L	122	SER	2.1
1	G	521	VAL	2.1
1	J	376	ARG	2.1
1	D	575	PRO	2.1
1	J	499	LYS	2.0
1	D	197	GLU	2.0
1	J	481	ALA	2.0
3	F	134	VAL	2.0
1	D	244	ILE	2.0
1	D	186	GLU	2.0
1	J	273	GLU	2.0
1	J	531	ASN	2.0
3	F	135	CYS	2.0
1	G	260	PHE	2.0
3	F	52	THR	2.0
1	J	570	TYR	2.0
1	J	355	GLY	2.0

## 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)

There are no ligands in this entry.



# 6.5 Other polymers (i)

There are no such residues in this entry.

