

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

#### Nov 15, 2023 – 03:55 PM JST

6JJL
Crystal structure of the DegP dodecamer with a modulator
Cho, H.; Choi, Y.; Lee, H.H.; Kim, S.
2019-02-26
4.20  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 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
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 4.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	$1005 \ (4.62-3.78)$
Clashscore	141614	$1044 \ (4.60-3.80)$
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain					
1	А	440	63%	22%	• 13%			
1	В	440	63%	24%	• 11%			
1	С	440	58%	28%	• 13%			
1	D	440	2% 57%	30%	• 12%			
1	Е	440	% 63%	24%	• 12%			
1	F	440	63%	22%	14%			



Mol Chain Length Quality of chain G 25100% 2Η 580% 20% 2 Ι 580% 20% J 25100% 2Κ 580% 20% L 52100% 25М 100% 2Ν 5100% 2Ο 5100% Р 52100% 2Q 5100% 2R 5100%

Continued from previous page...



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17212 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	Δ	381	Total	С	Ν	0	$\mathbf{S}$	0	0	0
1	Л	301	2791	1741	493	544	13	0	0	0
1	В	300	Total	С	Ν	0	S	0	0	0
1	D	592	2867	1783	506	565	13	0	0	0
1	С	380	Total	С	Ν	0	S	0	0	0
1		362	2794	1742	493	546	13		0	U
1	П	200	Total	С	Ν	0	S	0	0	0
1	D	300	2835	1766	499	557	13	0	0	
1	F	388	Total	С	Ν	0	S	0	0	0
1	Ľ	300	2835	1765	500	557	13	0	0	0
1	Б	270	Total	С	Ν	0	S	0	0	0
	Г	579	2777	1733	490	541	13	0		U

• Molecule 1 is a protein called Periplasmic serine endoprotease DegP.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	210	ALA	SER	conflict	UNP P0C0V0
В	210	ALA	SER	conflict	UNP P0C0V0
С	210	ALA	SER	conflict	UNP P0C0V0
D	210	ALA	SER	conflict	UNP P0C0V0
Е	210	ALA	SER	conflict	UNP P0C0V0
F	210	ALA	SER	conflict	UNP P0C0V0

• Molecule 2 is a protein called CYS-TYR-ARG-LYS-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total 25	C 15	N 5	O 5	0	0	0
2	М	5	Total 32	C 21	N 5	O 6	0	0	0
2	Н	5	Total 25	C 15	N 5	O 5	0	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Ν	5	Total         C         N         O           25         15         5         5	0	0	0
2	Ι	5	Total         C         N         O           28         18         5         5	0	0	0
2	Q	5	Total         C         N         O           25         15         5         5	0	0	0
2	J	5	Total         C         N         O           25         15         5         5	0	0	0
2	О	5	Total         C         N         O           25         15         5         5	0	0	0
2	K	5	Total         C         N         O           28         18         5         5	0	0	0
2	R	5	Total         C         N         O           25         15         5         5	0	0	0
2	L	5	Total         C         N         O           25         15         5         5	0	0	0
2	Р	5	Total         C         N         O           25         15         5         5	0	0	0

Continued from previous page...



# 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: Periplasmic serine endoprotease DegP

• Molecule 1: Periplasmic serine endoprotease DegP







# ASP L221 3864 L221 3864 T226 3775 L229 13776 L229 3777 L229 3776 L229 3777 L229 3776 L229 8377 L229 8377 L229 8377 L229 8377 L229 8377 L226 8387 L226 8387 L226 8388 L226 8387 L226 8389 L226 8389 L226 8389 L226 8389 L226 8386 L226 8386 L226 8389 L226 8389 L226 8399 L260 8400 L339 1310 L340 1407 L340 1408 L336 1446 L336 1446</t

• Molecule	1: Periplasmic serine endoprotease DegP			
Chain F:	63%	22%	14%	
ALA GLN Q11 L19 V22	S25 V27 V27 V27 V27 V27 V27 V37 V37 V37 V37 V37 V37 V37 V37 V37 V3	GLN GLN GLY SER PRO PRO GLN SER	SER PRO PHE CYS CYS GLN GLY GLN GLN	GLY ASN GLY GLY
GLY GLN GLN GLN M85 A86 A86 L87 L87	V1 15 V1 16 V1 15 V1 16 V1	N169 6172 176 176 177 1178	V182 R187 N191 N194 N194 F198	D202 1205
A213 L214 E220 L221 T222	1226 1226 1226 1226 1240 1242 1242 1242 1242 1265 1264 1265 1264 1265 1265 1265 1265 1265 1265 1265 1265	D308 V309 1310 T311 3311 S312 L313 L313 K316	P317 1318 5320 5320 R325 R325 P332	S335 K336 G340
L341 L342 R343 V350 N351 L352	<b>3357</b> SER ASN GLN VAL ASP ASP ASP F368 N369 N369 A374 A374 A374 C373 C373 C373 C373 C373 C373 C373 C	V415 K416 N417 1418 A419 E420 L421 L421 R422	D426 L432 L435 Q437 R438 R439	D440 L445 L446
M447 Q448				
• Molecule	2: CYS-TYR-ARG-LYS-LEU			
Chain G:	100%			
There are a	no outlier residues recorded for this chain.			
• Molecule	2: CYS-TYR-ARG-LYS-LEU			
Chain M:	100%			
There are a	no outlier residues recorded for this chain.			
• Molecule	2: CYS-TYR-ARG-LYS-LEU			
Chain H:	80%		20%	
C460				
• Molecule	2: CYS-TYR-ARG-LYS-LEU			
Chain N:	100%			
There are a	no outlier residues recorded for this chain.			

• Molecule 2: CYS-TYR-ARG-LYS-LEU



Chain I:	80%	20%
C460		
• Molecule 2: CYS-T	YR-ARG-LYS-LEU	
Chain Q:	100%	
There are no outlier r	esidues recorded for this chain.	
• Molecule 2: CYS-T	YR-ARG-LYS-LEU	
Chain J:	100%	
There are no outlier r	esidues recorded for this chain.	
• Molecule 2: CYS-T	YR-ARG-LYS-LEU	
Chain O:	100%	
There are no outlier r	residues recorded for this chain.	
• Molecule 2: CYS-T	YR-ARG-LYS-LEU	
Chain K:	80%	20%
C460		
• Molecule 2: CYS-T	YR-ARG-LYS-LEU	
Chain R:	100%	
There are no outlier r	esidues recorded for this chain.	
• Molecule 2: CYS-T	YR-ARG-LYS-LEU	
Chain L:	100%	
There are no outlier r	esidues recorded for this chain.	
• Molecule 2: CYS-T	YR-ARG-LYS-LEU	
Chain P:	100%	
There are no outlier r	esidues recorded for this chain.	



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	217.15Å 123.52Å 140.56Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $118.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	50.00 - 4.20	Depositor
Resolution (A)	40.67 - 4.16	EDS
% Data completeness	98.5(50.00-4.20)	Depositor
(in resolution range)	$98.7 \ (40.67 - 4.16)$	EDS
$R_{merge}$	0.11	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.08 (at 4.13 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
P. P.	0.248 , $0.326$	Depositor
$n, n_{free}$	0.255 , $0.328$	DCC
$R_{free}$ test set	1262 reflections $(5.15%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.24 , $44.2$	EDS
L-test for $twinning^2$	$<  L  > = 0.52, < L^2 > = 0.35$	Xtriage
	0.000 for $1/2$ *h- $3/2$ *k,- $1/2$ *h- $1/2$ *k,- $1/2$ *h	
Estimated twinning fraction	$+1/2^{*}k$ -l	Xtriage
0	0.000 for $1/2^{h+3}/2^{k}, 1/2^{h-1}/2^{k}, -1/2^{h-1}/2^{h-1}$	
E.E. correlation	1/2 <sup></sup> K-1	EDG
$\frac{\Gamma_{o}, \Gamma_{c} \text{ correlation}}{\text{Total number of stores}}$	0.04	
Access D all stores ( <sup>8</sup> 2)	<u> </u>	
Average B, all atoms $(A^2)$	52.0	WWPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.39% 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		
IVIOI	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.35	0/2815	0.51	0/3798	
1	В	0.34	0/2892	0.54	0/3904	
1	С	0.37	0/2818	0.54	0/3802	
1	D	0.31	0/2859	0.53	0/3858	
1	Ε	0.32	0/2859	0.52	0/3857	
1	F	0.33	0/2801	0.51	0/3779	
2	G	0.58	0/24	0.44	0/32	
2	Н	0.42	0/24	0.39	0/32	
2	Ι	0.37	0/27	0.69	0/36	
2	J	0.41	0/24	0.39	0/32	
2	Κ	0.37	0/27	0.66	0/36	
2	L	0.35	0/24	0.43	0/32	
2	М	0.36	0/32	0.42	0/43	
2	Ν	0.35	0/24	0.28	0/32	
2	0	0.33	0/24	0.32	0/32	
2	Р	0.26	0/24	0.30	0/32	
2	Q	0.33	0/24	0.40	0/32	
2	R	0.32	0/24	0.44	0/32	
All	All	0.34	0/17346	0.52	0/23401	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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



6.	IJ	Ľ
0.	,0	-

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2791	0	2888	63	1
1	В	2867	0	2957	75	0
1	С	2794	0	2890	100	0
1	D	2835	0	2929	111	0
1	Ε	2835	0	2929	87	0
1	F	2777	0	2875	51	0
2	G	25	0	9	0	0
2	Н	25	0	9	1	0
2	Ι	28	0	18	1	0
2	J	25	0	9	0	0
2	K	28	0	18	5	0
2	L	25	0	9	0	0
2	М	32	0	16	0	0
2	N	25	0	9	0	0
2	0	25	0	9	0	0
2	Р	25	0	9	0	0
2	Q	25	0	9	0	0
2	R	25	0	9	0	0
All	All	17212	0	17601	466	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 13.

All (466) 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:D:387:VAL:HG21	1:D:405:ASP:H	1.14	1.10
1:D:305:LYS:HD3	1:D:343:ARG:NH2	1.84	0.93
1:E:82:GLN:HG2	1:E:83:LYS:HA	1.56	0.88
1:B:408:ILE:H	1:B:409:GLY:HA3	1.37	0.88
1:B:409:GLY:HA2	1:B:435:ASN:HB3	1.57	0.87
1:D:407:ILE:HG13	1:D:408:ILE:HG22	1.57	0.85
1:D:246:MET:HG2	1:D:330:THR:HG21	1.58	0.84
1:D:387:VAL:HG13	1:D:406:VAL:HG23	1.62	0.82
1:D:374:ALA:HB1	1:D:389:ASN:HB2	1.61	0.82
1:D:187:ARG:NH1	1:D:200:GLN:OE1	2.15	0.80
1:C:436:ILE:HG22	1:C:437:GLN:H	1.45	0.79
1:C:435:ASN:ND2	1:C:443:ILE:O	2.16	0.79
1:E:318:ILE:HD11	1:E:324:LEU:HB2	1.64	0.78
1:E:34:SER:HA	1:E:82:GLN:HG3	1.63	0.78
1:C:318:ILE:HD12	1:C:324:LEU:HD13	1.66	0.76
1:E:402:LYS:HE3	1:E:438:ARG:HD3	1.68	0.76



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:215:VAL:HG12	1:B:221:LEU:HA	1.67	0.75
1:C:35:THR:HG22	1:C:84:PHE:HB3	1.69	0.74
1:D:387:VAL:HG21	1:D:405:ASP:N	1.98	0.73
1:C:407:ILE:HA	1:C:436:ILE:HG12	1.71	0.73
1:C:92:ILE:HG22	1:C:100:VAL:HB	1.71	0.73
1:B:22:VAL:HG21	1:B:219:GLY:HA3	1.72	0.71
1:C:435:ASN:CG	1:C:444:TYR:HA	2.11	0.71
1:D:308:ASP:OD1	1:D:343:ARG:HA	1.90	0.71
1:D:268:MET:HB2	1:D:292:GLN:HB3	1.72	0.71
1:D:32:GLU:HG3	1:D:85:MET:HG2	1.73	0.70
1:D:407:ILE:HD13	1:D:437:GLN:HG2	1.73	0.70
1:E:19:LEU:HD21	1:E:177:VAL:HG11	1.74	0.70
1:D:305:LYS:HD3	1:D:343:ARG:HH22	1.57	0.69
1:E:262:ARG:NH1	1:E:329:GLY:O	2.26	0.69
1:C:195:TYR:HD2	1:C:326:ALA:HA	1.58	0.68
1:E:215:VAL:HG12	1:E:221:LEU:HA	1.75	0.68
1:F:304:ILE:HG23	1:F:341:LEU:HD21	1.74	0.68
1:D:407:ILE:HB	1:D:436:ILE:HA	1.76	0.68
1:E:386:VAL:HA	1:E:406:VAL:HG23	1.75	0.68
1:D:31:VAL:HG23	1:D:113:ILE:HG12	1.76	0.68
1:C:169:ASN:HD21	1:C:172:GLY:HA2	1.58	0.67
1:C:380:GLY:O	1:C:383:GLN:NE2	2.28	0.67
1:C:386:VAL:HG22	1:C:406:VAL:HA	1.74	0.67
1:B:376:MET:HG2	1:B:387:VAL:HG22	1.75	0.67
1:A:187:ARG:NH1	1:A:200:GLN:OE1	2.27	0.67
1:B:328:VAL:HA	1:B:331:MET:HG3	1.76	0.67
1:C:265:LEU:HD11	1:C:352:LEU:HD13	1.77	0.66
1:B:374:ALA:H	1:B:396:ALA:HB3	1.61	0.66
1:A:129:GLY:HA3	1:A:254:MET:HG2	1.77	0.66
1:E:415:VAL:HG13	1:E:420:GLU:HB3	1.77	0.66
1:D:305:LYS:HB2	1:D:343:ARG:HH12	1.61	0.66
1:C:370:GLY:HA2	1:C:376:MET:HG2	1.79	0.65
1:C:411:ASN:N	1:C:434:LEU:HD11	2.12	0.65
1:E:288:ALA:HB3	1:E:310:ILE:HB	1.77	0.65
1:A:23:MET:HG2	1:A:175:GLU:OE1	1.96	0.65
1:E:384:GLY:HA3	1:E:416:LYS:O	1.96	0.65
1:C:103:ASN:HD22	1:C:104:ASN:N	1.94	0.65
1:B:408:ILE:N	1:B:409:GLY:HA3	2.11	0.65
1:C:178:THR:HG21	1:C:204:ALA:HB3	1.78	0.65
1:B:205:ILE:O	1:B:235:ASN:HB2	1.96	0.64
1:E:422:ARG:HA	1:E:425:LEU:HB3	1.79	0.64



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:158:LEU:HD11	1:C:222:ILE:HD12	1.80	0.64
1:C:136:ILE:HD13	1:C:247:VAL:HG13	1.80	0.64
1:C:407:ILE:HA	1:C:436:ILE:CG1	2.28	0.64
1:D:385:VAL:N	1:D:406:VAL:HG11	2.13	0.64
1:F:31:VAL:HB	1:F:86:ALA:HB3	1.81	0.64
1:A:379:LYS:HE2	1:A:406:VAL:HG22	1.80	0.63
1:D:178:THR:HG21	1:D:204:ALA:HB3	1.79	0.63
1:D:263:GLY:HA3	1:D:354:LEU:HD12	1.79	0.63
1:B:374:ALA:HB2	1:B:390:VAL:HG23	1.79	0.63
1:E:399:ILE:HD13	1:E:401:LEU:HG	1.80	0.63
1:A:178:THR:HG21	1:A:204:ALA:HB3	1.80	0.63
1:D:124:ASP:HB3	1:D:142:GLN:HG3	1.81	0.63
1:E:102:THR:HG23	1:E:137:ALA:HB3	1.81	0.63
1:C:435:ASN:ND2	1:C:444:TYR:HA	2.14	0.62
1:D:312:SER:HB3	1:D:340:GLY:HA3	1.80	0.62
1:D:103:ASN:HD21	1:D:226:THR:HG22	1.65	0.62
1:C:102:THR:OG1	1:C:103:ASN:N	2.32	0.62
1:A:298:SER:OG	1:A:355:GLN:NE2	2.32	0.62
1:C:385:VAL:HB	1:C:407:ILE:HD12	1.81	0.62
1:A:205:ILE:HG23	1:A:209:ASN:HB2	1.82	0.62
1:C:411:ASN:H	1:C:434:LEU:HD11	1.62	0.62
1:A:422:ARG:O	1:A:426:ASP:N	2.28	0.61
1:E:408:ILE:HG12	1:E:421:LEU:HD21	1.81	0.61
1:F:19:LEU:HA	1:F:22:VAL:HG12	1.81	0.61
1:C:29:ILE:HG22	1:C:30:ASN:H	1.64	0.61
1:F:91:VAL:HG21	1:F:213:ALA:HB2	1.81	0.61
1:F:265:LEU:HD22	1:F:352:LEU:HD13	1.82	0.61
1:A:332:PRO:O	1:A:335:SER:OG	2.17	0.61
1:B:19:LEU:HB3	1:B:23:MET:HG3	1.82	0.61
1:B:202:ASP:HA	1:B:237:GLY:O	2.00	0.61
1:C:408:ILE:HB	1:C:436:ILE:HG23	1.82	0.61
1:D:405:ASP:OD1	1:D:437:GLN:N	2.34	0.60
1:E:261:LYS:HE2	1:E:333:VAL:HB	1.82	0.60
1:B:178:THR:HG22	1:C:202:ASP:HB3	1.83	0.60
1:E:206:ASN:C	2:K:464:LEU:HD12	2.20	0.60
1:B:407:ILE:HD13	1:B:434:LEU:HD22	1.84	0.60
1:C:408:ILE:N	1:C:436:ILE:HG12	2.17	0.60
1:D:12:MET:SD	1:E:216:ASN:ND2	2.73	0.60
1:D:305:LYS:HB2	1:D:343:ARG:NH1	2.16	0.60
1:D:290:VAL:HG13	1:D:310:ILE:HD11	1.84	0.60
1:D:176:THR:HG22	1:E:187:ARG:HH12	1.67	0.59



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:158:LEU:HD11	1:D:222:ILE:HD12	1.84	0.59
1:D:310:ILE:HG21	1:D:339:LEU:HD22	1.83	0.59
1:C:103:ASN:HB3	1:C:106:VAL:HG23	1.85	0.59
1:C:86:ALA:HB1	1:C:207:ARG:HH22	1.68	0.58
1:C:341:LEU:HB3	1:C:348:VAL:HG23	1.84	0.58
1:A:328:VAL:HA	1:A:331:MET:HG3	1.84	0.58
1:A:388:ASN:O	1:A:389:ASN:ND2	2.36	0.58
1:C:411:ASN:H	1:C:434:LEU:CD1	2.16	0.58
1:D:143:ASN:HB3	1:D:145:LYS:HE2	1.86	0.58
1:C:389:ASN:HA	1:C:403:LYS:HG2	1.86	0.58
1:C:408:ILE:H	1:C:436:ILE:HG12	1.68	0.58
1:B:127:MET:HA	1:B:139:ILE:HG22	1.86	0.57
1:B:367:ILE:O	1:B:422:ARG:NH1	2.37	0.57
1:C:160:VAL:HG23	1:C:185:LEU:HG	1.85	0.57
1:A:150:ILE:HD13	1:A:221:LEU:HB2	1.85	0.57
1:E:20:GLU:OE1	1:F:159:ARG:NH2	2.37	0.57
1:E:178:THR:HG22	1:F:202:ASP:HB3	1.85	0.57
1:E:187:ARG:NH1	1:E:200:GLN:OE1	2.36	0.57
1:F:304:ILE:HD11	1:F:352:LEU:HD11	1.85	0.57
1:B:210:ALA:HB2	2:H:464:LEU:O	2.04	0.57
1:B:242:ILE:HG23	1:B:246:MET:HE2	1.87	0.57
1:A:181:ILE:HD13	1:C:179:SER:HB3	1.87	0.57
1:E:399:ILE:HD12	1:E:400:GLY:N	2.19	0.57
1:E:243:PRO:O	1:E:247:VAL:HG23	2.05	0.57
1:F:408:ILE:HD13	1:F:437:GLN:HG3	1.85	0.57
1:A:407:ILE:HG12	1:A:436:ILE:HG22	1.86	0.56
1:D:390:VAL:HG22	1:D:403:LYS:HB3	1.86	0.56
1:E:408:ILE:HD13	1:E:416:LYS:HA	1.87	0.56
1:D:407:ILE:HG21	1:D:435:ASN:HB3	1.87	0.56
1:E:103:ASN:O	1:E:106:VAL:HG12	2.05	0.56
1:E:261:LYS:HG3	1:E:333:VAL:H	1.69	0.56
1:A:215:VAL:HG12	1:A:221:LEU:HA	1.87	0.56
1:A:183:SER:HB2	1:A:200:GLN:HG2	1.87	0.56
1:D:385:VAL:HG12	1:D:386:VAL:H	1.70	0.56
1:A:179:SER:HB2	1:B:181:ILE:HD13	1.88	0.56
1:F:288:ALA:HB3	1:F:310:ILE:HB	1.87	0.56
1:D:215:VAL:HG12	1:D:221:LEU:HA	1.86	0.56
1:A:379:LYS:HD3	1:A:386:VAL:HB	1.87	0.56
1:B:246:MET:O	1:B:250:LEU:HD12	2.06	0.56
1:E:386:VAL:HA	1:E:406:VAL:CG2	2.35	0.55
1:D:179:SER:HB3	1:E:181:ILE:HD13	1.89	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:30:ASN:HA	1:C:87:LEU:HD13	1.89	0.55
1:E:379:LYS:HA	1:E:384:GLY:HA2	1.89	0.55
1:D:313:LEU:HB2	1:D:318:ILE:HD11	1.89	0.55
1:E:407:ILE:HG13	1:E:436:ILE:HA	1.88	0.55
1:B:281:LYS:HE2	1:D:412:GLN:HG3	1.89	0.54
1:B:292:GLN:HB3	1:D:443:ILE:HB	1.89	0.54
1:F:407:ILE:HG12	1:F:436:ILE:HG22	1.90	0.54
1:F:386:VAL:HG22	1:F:406:VAL:HG22	1.90	0.54
1:A:205:ILE:HG23	1:A:209:ASN:CB	2.37	0.54
1:C:406:VAL:O	1:C:436:ILE:HD13	2.07	0.54
1:B:363:ASP:OD1	1:B:375:GLU:HB3	2.08	0.54
1:F:253:GLN:OE1	1:F:261:LYS:N	2.41	0.54
1:D:407:ILE:HG21	1:D:435:ASN:C	2.28	0.54
1:C:371:ILE:HD13	1:C:421:LEU:HD21	1.90	0.54
1:D:183:SER:N	1:D:200:GLN:O	2.41	0.54
1:E:29:ILE:HG22	1:E:115:VAL:HG22	1.90	0.54
1:E:31:VAL:HG12	1:E:113:ILE:HG12	1.90	0.53
1:A:205:ILE:O	1:A:235:ASN:HB2	2.08	0.53
1:F:103:ASN:ND2	1:F:135:ASP:O	2.39	0.53
1:C:407:ILE:HA	1:C:436:ILE:CD1	2.37	0.53
1:E:102:THR:OG1	1:E:103:ASN:N	2.41	0.53
1:F:169:ASN:OD1	1:F:172:GLY:HA2	2.09	0.53
1:B:104:ASN:ND2	1:B:135:ASP:HA	2.24	0.53
1:D:399:ILE:HB	1:D:445:LEU:HD21	1.91	0.53
1:E:399:ILE:HD12	1:E:400:GLY:H	1.74	0.53
1:E:364:SER:N	1:E:376:MET:HG2	2.24	0.53
1:C:406:VAL:HG12	1:C:407:ILE:H	1.74	0.53
1:A:133:ARG:HB3	1:A:195:TYR:CE2	2.44	0.52
1:D:436:ILE:O	1:D:443:ILE:HG12	2.08	0.52
1:D:354:LEU:HD23	1:D:354:LEU:H	1.74	0.52
1:F:158:LEU:HD22	1:F:182:VAL:HG21	1.90	0.52
1:B:121:ARG:HA	1:C:285:GLN:HG2	1.91	0.52
1:D:408:ILE:CG1	1:D:414:ALA:HA	2.39	0.52
1:D:299:ALA:HA	1:D:352:LEU:HD21	1.89	0.52
1:B:35:THR:N	1:B:82:GLN:O	2.43	0.52
1:E:18:MET:SD	1:E:19:LEU:HD12	2.50	0.52
1:E:379:LYS:HE3	1:E:417:ASN:HB2	1.92	0.52
1:D:286:ARG:NH2	1:F:118:SER:O	2.42	0.52
1:B:119:ASP:HB2	1:B:121:ARG:HG3	1.91	0.52
1:E:387:VAL:HG13	1:E:406:VAL:HG21	1.92	0.51
1:D:22:VAL:HG21	1:D:219:GLY:HA3	1.92	0.51



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:368:PHE:CG	1:D:372:GLU:HA	2.46	0.51
1:A:391:LYS:O	1:A:394:THR:OG1	2.28	0.51
1:D:382:ASP:O	1:D:416:LYS:HB2	2.11	0.51
1:D:33:GLY:HA2	1:D:110:ALA:HA	1.91	0.51
1:F:432:LEU:O	1:F:446:LEU:HA	2.10	0.51
1:A:272:LEU:HD11	1:A:277:ALA:HB2	1.91	0.51
1:F:108:ASP:OD1	1:F:130:LYS:NZ	2.36	0.51
1:A:353:GLU:HG3	1:A:354:LEU:O	2.10	0.51
1:E:104:ASN:HA	1:E:137:ALA:HB2	1.92	0.51
1:D:399:ILE:O	1:D:445:LEU:HD11	2.11	0.51
1:D:406:VAL:CG1	1:D:407:ILE:N	2.74	0.51
1:E:178:THR:HG21	1:E:204:ALA:HB3	1.91	0.51
1:F:332:PRO:O	1:F:335:SER:OG	2.26	0.51
1:D:24:PRO:HA	1:D:118:SER:HB3	1.92	0.50
1:D:126:LYS:H	1:D:126:LYS:HD2	1.76	0.50
1:C:438:ARG:CZ	1:C:443:ILE:HD11	2.41	0.50
1:E:207:ARG:HA	2:K:464:LEU:HB2	1.93	0.50
1:B:443:ILE:HG22	1:B:444:TYR:N	2.25	0.50
1:E:100:VAL:HB	1:E:139:ILE:HG13	1.93	0.50
1:B:288:ALA:HB1	1:B:321:PHE:HD1	1.76	0.50
1:D:186:GLY:HA2	1:D:197:ASN:OD1	2.11	0.50
1:A:250:LEU:HG	1:A:330:THR:HG23	1.93	0.50
1:C:32:GLU:HB2	1:C:112:VAL:HG12	1.93	0.50
1:B:222:ILE:O	1:B:244:SER:N	2.44	0.50
1:D:420:GLU:HA	1:D:423:LYS:HE2	1.93	0.50
1:E:423:LYS:HE2	1:E:424:VAL:HG23	1.94	0.50
1:B:164:THR:HB	1:B:214:LEU:HD21	1.93	0.50
1:C:155:SER:N	1:C:245:ASN:OD1	2.45	0.50
1:C:379:LYS:HD3	1:C:386:VAL:HB	1.94	0.50
1:C:86:ALA:HB1	1:C:207:ARG:NH2	2.26	0.50
1:D:408:ILE:HG23	1:D:409:GLY:H	1.77	0.50
1:A:257:TYR:CD1	1:A:257:TYR:N	2.80	0.49
1:D:406:VAL:HG12	1:D:407:ILE:N	2.28	0.49
1:A:127:MET:SD	1:A:130:LYS:HE3	2.52	0.49
1:D:374:ALA:HB1	1:D:389:ASN:CB	2.39	0.49
1:E:405:ASP:O	1:E:406:VAL:HG13	2.11	0.49
1:A:249:ASN:HB2	1:A:330:THR:CG2	2.42	0.49
1:C:261:LYS:HB3	1:C:333:VAL:HG23	1.93	0.49
1:E:226:THR:O	2:K:464:LEU:HD23	2.13	0.49
1:E:407:ILE:HG12	1:E:437:GLN:HG2	1.93	0.49
1:C:88:GLY:HA2	1:C:208:GLY:HA2	1.94	0.49



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:422:ARG:O	1:C:426:ASP:N	2.45	0.49
1:D:272:LEU:HD22	1:D:309:VAL:HG11	1.95	0.49
1:D:313:LEU:HD11	1:D:337:LEU:HD23	1.95	0.49
1:E:121:ARG:NH1	1:E:145:LYS:O	2.36	0.49
1:E:384:GLY:C	1:E:408:ILE:HD11	2.32	0.49
1:D:178:THR:HG21	1:D:204:ALA:H	1.78	0.49
1:C:29:ILE:HG22	1:C:30:ASN:N	2.26	0.48
1:C:100:VAL:HG13	1:C:139:ILE:HG13	1.94	0.48
1:A:102:THR:OG1	1:A:103:ASN:N	2.47	0.48
1:C:385:VAL:N	1:C:407:ILE:HB	2.28	0.48
1:A:327:GLN:O	1:A:330:THR:HB	2.13	0.48
1:B:104:ASN:HD22	1:B:135:ASP:HA	1.78	0.48
1:D:27:VAL:HG12	1:D:117:LEU:HA	1.95	0.48
1:D:408:ILE:HG13	1:D:414:ALA:HA	1.96	0.48
1:D:435:ASN:O	1:D:435:ASN:ND2	2.46	0.48
1:A:290:VAL:HG22	1:A:308:ASP:O	2.14	0.48
1:B:378:ASN:HD21	1:B:418:ILE:H	1.62	0.48
1:E:136:ILE:HD11	1:E:247:VAL:HG22	1.96	0.48
1:A:127:MET:HA	1:A:139:ILE:HG22	1.95	0.47
1:D:373:GLY:HA3	1:D:396:ALA:HB3	1.96	0.47
1:D:385:VAL:H	1:D:406:VAL:HG11	1.78	0.47
1:C:166:ALA:N	1:C:178:THR:O	2.33	0.47
1:D:155:SER:N	1:D:245:ASN:OD1	2.46	0.47
1:C:162:ASP:O	1:C:182:VAL:HG23	2.14	0.47
1:C:410:ALA:HA	1:C:434:LEU:HD12	1.97	0.47
1:C:433:ALA:N	1:C:434:LEU:HD22	2.29	0.47
1:B:179:SER:HB3	1:C:181:ILE:HD13	1.97	0.47
1:C:396:ALA:HA	1:C:399:ILE:HD12	1.97	0.47
1:D:119:ASP:HB3	1:D:121:ARG:HG3	1.95	0.47
1:A:318:ILE:HD11	1:A:324:LEU:HD13	1.96	0.47
1:B:308:ASP:OD2	1:B:343:ARG:NH2	2.48	0.47
1:C:150:ILE:HD13	1:C:221:LEU:HB2	1.96	0.47
1:C:407:ILE:HA	1:C:436:ILE:HD13	1.97	0.47
1:E:250:LEU:O	1:E:254:MET:HG3	2.14	0.47
1:E:387:VAL:HG23	1:E:403:LYS:HA	1.97	0.47
1:F:187:ARG:HA	1:F:187:ARG:HD3	1.56	0.47
1:B:150:ILE:HD11	1:B:215:VAL:HG11	1.97	0.47
1:A:23:MET:N	1:A:24:PRO:HD2	2.30	0.46
1:F:308:ASP:OD1	1:F:343:ARG:HB3	2.14	0.46
1:A:25:SER:OG	1:A:150:ILE:HB	2.15	0.46
1:C:293:VAL:HG11	1:C:304:ILE:O	2.15	0.46



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:391:LYS:HG2	1:C:394:THR:HG23	1.97	0.46
1:E:282:VAL:HG12	1:E:284:ALA:H	1.80	0.46
1:C:266:GLY:HA3	1:C:297:SER:OG	2.15	0.46
1:B:178:THR:HG21	1:B:204:ALA:HB3	1.98	0.46
1:D:407:ILE:HG12	1:D:435:ASN:O	2.15	0.46
1:E:138:LEU:HB3	1:E:254:MET:HE2	1.98	0.46
1:B:271:GLU:HG3	1:B:321:PHE:H	1.79	0.46
1:C:153:ALA:HB2	1:C:220:GLU:HB2	1.98	0.46
1:E:195:TYR:HB3	1:E:326:ALA:HA	1.96	0.46
1:C:103:ASN:ND2	1:C:135:ASP:O	2.49	0.46
1:D:387:VAL:HG11	1:D:405:ASP:O	2.16	0.46
1:B:19:LEU:HD11	1:B:177:VAL:HG11	1.97	0.46
1:B:440:ASP:N	1:B:440:ASP:OD1	2.48	0.46
1:C:324:LEU:O	1:C:328:VAL:HG22	2.16	0.46
1:E:127:MET:HA	1:E:139:ILE:HG22	1.98	0.46
1:B:431:VAL:HA	1:B:448:GLN:CD	2.37	0.46
1:D:335:SER:H	1:D:354:LEU:HD21	1.80	0.46
1:C:262:ARG:HD3	1:C:329:GLY:O	2.16	0.46
1:E:377:SER:N	1:E:386:VAL:O	2.43	0.46
1:E:401:LEU:HD22	1:E:445:LEU:HD13	1.97	0.46
1:C:288:ALA:HB1	1:C:321:PHE:HD2	1.81	0.46
1:D:297:SER:O	1:D:301:LYS:HG3	2.16	0.46
1:D:365:SER:HA	1:D:368:PHE:HD2	1.80	0.46
1:A:187:ARG:HA	1:A:187:ARG:HD3	1.77	0.45
1:C:183:SER:N	1:C:200:GLN:O	2.48	0.45
1:C:436:ILE:HG22	1:C:437:GLN:N	2.22	0.45
1:D:183:SER:HB3	1:F:176:THR:HG23	1.98	0.45
1:E:210:ALA:HB2	2:K:464:LEU:C	2.36	0.45
1:B:267:ILE:HD13	1:B:299:ALA:HB3	1.98	0.45
1:D:407:ILE:HG23	1:D:408:ILE:C	2.37	0.45
1:E:338:THR:O	1:E:339:LEU:HD23	2.17	0.45
1:E:379:LYS:HZ2	1:E:418:ILE:HB	1.82	0.45
1:A:298:SER:HA	1:A:301:LYS:HE2	1.98	0.45
1:B:371:ILE:HG21	1:B:447:MET:HE1	1.98	0.45
1:A:288:ALA:HB3	1:A:310:ILE:HB	1.99	0.45
1:A:288:ALA:O	1:A:309:VAL:HA	2.17	0.45
1:D:234:GLY:O	1:D:236:ILE:HG23	2.17	0.45
1:D:202:ASP:HB3	1:F:178:THR:HG22	1.98	0.45
1:B:204:ALA:HA	1:B:235:ASN:OD1	2.17	0.45
1:C:92:ILE:HA	1:C:100:VAL:HA	1.99	0.45
1:D:83:LYS:HB2	1:D:83:LYS:HE3	1.79	0.45



	i a pageini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:19:LEU:HD21	1:C:165:VAL:HG11	1.99	0.45
1:C:272:LEU:HD21	1:C:284:ALA:O	2.17	0.45
1:D:387:VAL:CG2	1:D:405:ASP:H	2.04	0.45
1:F:102:THR:OG1	1:F:103:ASN:N	2.50	0.45
1:A:173:LEU:HD11	1:B:229:LEU:HD23	1.99	0.44
1:C:246:MET:HE3	1:C:330:THR:HG21	1.99	0.44
1:C:435:ASN:C	1:C:436:ILE:HG13	2.36	0.44
1:F:103:ASN:HD21	1:F:226:THR:HG23	1.82	0.44
1:F:395:PRO:O	1:F:399:ILE:HG23	2.17	0.44
1:B:378:ASN:HD21	1:B:417:ASN:HB2	1.82	0.44
1:C:271:GLU:OE2	1:C:320:SER:HB2	2.17	0.44
1:D:19:LEU:HB3	1:D:23:MET:SD	2.57	0.44
1:B:176:THR:HG23	1:C:183:SER:HB3	2.00	0.44
1:C:304:ILE:HA	1:C:343:ARG:HH22	1.82	0.44
1:C:131:ASP:HB2	1:C:260:VAL:HG21	1.98	0.44
1:E:136:ILE:HD12	1:E:250:LEU:HD12	1.99	0.44
1:B:130:LYS:O	1:B:132:PRO:HD3	2.18	0.44
1:C:328:VAL:HG12	1:C:331:MET:SD	2.57	0.44
1:D:226:THR:HG21	1:D:242:ILE:HD12	2.00	0.44
1:E:198:PHE:CD2	1:E:240:PHE:HB3	2.53	0.44
1:F:374:ALA:HB1	1:F:387:VAL:HG13	2.00	0.44
1:F:440:ASP:OD1	1:F:440:ASP:N	2.48	0.44
1:B:150:ILE:HD13	1:B:221:LEU:HB2	2.00	0.44
1:B:223:GLY:HA2	1:B:242:ILE:O	2.18	0.44
1:B:416:LYS:HE3	1:B:420:GLU:OE2	2.18	0.44
1:C:425:LEU:HD21	1:C:432:LEU:HD11	1.99	0.44
1:A:195:TYR:HD1	1:A:326:ALA:HA	1.83	0.43
1:C:168:GLY:O	1:C:175:GLU:HA	2.18	0.43
1:C:415:VAL:HG23	1:C:420:GLU:HB2	2.00	0.43
1:D:387:VAL:HG23	1:D:404:GLY:H	1.83	0.43
1:E:379:LYS:NZ	1:E:418:ILE:HB	2.32	0.43
1:F:311:THR:O	1:F:318:ILE:HG22	2.17	0.43
1:B:435:ASN:HB2	1:B:444:TYR:CZ	2.53	0.43
1:E:308:ASP:OD1	1:E:343:ARG:HG2	2.19	0.43
1:A:373:GLY:HA2	1:A:395:PRO:HD2	2.00	0.43
1:D:402:LYS:HD2	1:D:402:LYS:C	2.37	0.43
1:E:104:ASN:HB3	1:E:135:ASP:HA	1.99	0.43
1:D:280:MET:HB3	1:D:282:VAL:HG23	1.99	0.43
1:F:445:LEU:HD23	1:F:445:LEU:HA	1.79	0.43
1:C:92:ILE:HG13	1:C:149:ALA:HA	1.99	0.43
1:E:158:LEU:HD22	1:E:182:VAL:HG21	2.01	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:417:ASN:ND2	1:F:419:ALA:HB3	2.34	0.43
1:B:205:ILE:HG23	1:B:209:ASN:HB3	2.01	0.43
1:F:205:ILE:HD13	1:F:225:ASN:HB3	1.99	0.43
1:F:415:VAL:HG21	1:F:421:LEU:HB2	2.01	0.43
1:A:158:LEU:HD11	1:A:222:ILE:HD12	2.00	0.43
1:A:183:SER:N	1:A:200:GLN:O	2.51	0.43
1:A:251:THR:HA	1:A:254:MET:HB2	2.00	0.43
1:B:379:LYS:HD3	1:B:379:LYS:HA	1.72	0.43
1:E:205:ILE:HG23	1:E:209:ASN:HB3	2.01	0.43
1:E:389:ASN:HA	1:E:403:LYS:HD2	2.00	0.43
1:C:169:ASN:O	1:C:169:ASN:ND2	2.52	0.43
1:D:409:GLY:O	1:D:435:ASN:HB2	2.19	0.43
1:F:312:SER:OG	1:F:340:GLY:HA3	2.19	0.43
1:B:281:LYS:HE3	1:B:281:LYS:HB2	1.92	0.43
1:C:435:ASN:O	1:C:436:ILE:HG13	2.19	0.43
1:A:249:ASN:HB2	1:A:330:THR:HG22	1.99	0.43
1:A:272:LEU:HD22	1:A:309:VAL:HG11	1.99	0.43
1:D:343:ARG:HG3	1:D:344:ASP:H	1.83	0.43
1:F:126:LYS:HE2	1:F:126:LYS:HB3	1.87	0.43
1:A:313:LEU:HD22	1:A:324:LEU:HD12	2.00	0.42
1:A:343:ARG:HD2	1:A:348:VAL:HG21	2.01	0.42
1:B:232:ASP:OD1	1:B:232:ASP:N	2.50	0.42
1:A:308:ASP:OD2	1:A:343:ARG:NH1	2.52	0.42
1:B:250:LEU:O	1:B:254:MET:HG3	2.19	0.42
1:B:269:GLY:HA3	1:B:289:PHE:O	2.20	0.42
1:C:119:ASP:OD1	1:C:119:ASP:N	2.50	0.42
1:C:197:ASN:O	1:C:197:ASN:ND2	2.51	0.42
1:F:416:LYS:HB2	1:F:417:ASN:H	1.74	0.42
1:B:104:ASN:CB	1:B:137:ALA:HB2	2.49	0.42
1:F:153:ALA:HB2	1:F:220:GLU:HB3	2.00	0.42
1:A:176:THR:HG21	1:B:200:GLN:HE22	1.85	0.42
1:C:99:TYR:HE1	1:C:140:GLN:OE1	2.01	0.42
1:C:274:SER:HA	1:C:285:GLN:HG3	2.01	0.42
1:E:309:VAL:O	1:E:341:LEU:HA	2.20	0.42
1:E:436:ILE:HD11	1:E:438:ARG:HE	1.83	0.42
1:A:374:ALA:HB1	1:A:390:VAL:HA	2.00	0.42
1:B:87:LEU:HD12	1:B:87:LEU:O	2.20	0.42
1:B:443:ILE:CG2	1:B:444:TYR:N	2.83	0.42
1:C:210:ALA:HB2	2:I:464:LEU:O	2.19	0.42
1:C:246:MET:HE3	1:C:246:MET:HB3	1.89	0.42
1:D:264:GLU:HB2	1:D:357:SER:HA	2.01	0.42



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:205:ILE:HG22	2:K:464:LEU:HD11	2.02	0.42
1:B:31:VAL:O	1:B:85:MET:HA	2.19	0.42
1:D:156:ASP:HB3	1:D:316:LYS:HE2	2.01	0.42
1:D:385:VAL:HG12	1:D:386:VAL:N	2.35	0.42
1:D:267:ILE:HD12	1:D:290:VAL:HG12	2.01	0.42
1:E:308:ASP:CG	1:E:343:ARG:HG2	2.39	0.42
1:E:405:ASP:C	1:E:406:VAL:HG13	2.40	0.42
1:B:421:LEU:HG	1:B:425:LEU:HD11	2.02	0.42
1:C:30:ASN:OD1	1:C:87:LEU:HD22	2.20	0.42
1:D:121:ARG:HG2	1:E:285:GLN:HG2	2.01	0.42
1:D:352:LEU:HD23	1:D:352:LEU:HA	1.89	0.42
1:E:205:ILE:O	1:E:235:ASN:HB2	2.20	0.42
1:A:31:VAL:HG21	1:A:107:VAL:HG23	2.02	0.41
1:A:133:ARG:HB3	1:A:195:TYR:CD2	2.55	0.41
1:B:341:LEU:HB3	1:B:348:VAL:HG23	2.02	0.41
1:D:323:ALA:O	1:D:327:GLN:N	2.47	0.41
1:D:326:ALA:O	1:D:330:THR:HG22	2.19	0.41
1:E:399:ILE:HG22	1:E:447:MET:CE	2.50	0.41
1:B:16:ALA:N	1:B:17:PRO:HD2	2.35	0.41
1:B:19:LEU:CD1	1:B:177:VAL:HG11	2.50	0.41
1:C:29:ILE:C	1:C:87:LEU:HD11	2.40	0.41
1:C:407:ILE:HG12	1:C:436:ILE:HD13	2.01	0.41
1:D:150:ILE:HD13	1:D:221:LEU:HB2	2.02	0.41
1:D:168:GLY:HA3	1:D:209:ASN:HD22	1.86	0.41
1:D:379:LYS:HE2	1:D:383:GLN:HB2	2.01	0.41
1:E:385:VAL:HG22	1:E:418:ILE:HG12	2.02	0.41
1:B:183:SER:HB2	1:B:200:GLN:HG2	2.02	0.41
1:D:163:TYR:HB2	1:D:217:LEU:HD11	2.02	0.41
1:D:407:ILE:HG13	1:D:408:ILE:H	1.85	0.41
1:A:150:ILE:HG12	1:A:151:LYS:O	2.21	0.41
1:C:250:LEU:O	1:C:254:MET:HG3	2.19	0.41
1:C:342:LEU:HD12	1:C:342:LEU:HA	1.87	0.41
1:E:88:GLY:HA3	1:E:106:VAL:HG21	2.02	0.41
1:E:387:VAL:CG2	1:E:403:LYS:HA	2.50	0.41
1:F:290:VAL:HG23	1:F:308:ASP:O	2.18	0.41
1:A:227:ALA:O	1:A:240:PHE:N	2.54	0.41
1:B:133:ARG:HG3	1:B:262:ARG:HH21	1.86	0.41
1:F:422:ARG:O	1:F:426:ASP:N	2.40	0.41
1:A:152:MET:CE	1:A:248:LYS:HB2	2.51	0.41
1:B:117:LEU:HD11	1:B:147:LEU:HD22	2.03	0.41
1:D:407:ILE:HG13	1:D:408:ILE:N	2.36	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:379:LYS:CA	1:E:384:GLY:HA2	2.51	0.41
1:E:405:ASP:OD1	1:E:406:VAL:N	2.53	0.41
1:D:173:LEU:HD11	1:E:229:LEU:HD23	2.02	0.41
1:F:191:ASN:HB3	1:F:194:ASN:HB2	2.02	0.41
1:A:174:GLY:O	1:A:176:THR:HG23	2.21	0.41
1:A:228:ILE:O	1:A:228:ILE:HG13	2.21	0.41
1:D:341:LEU:HB2	1:D:348:VAL:O	2.21	0.41
1:F:368:PHE:CE2	1:F:422:ARG:HD3	2.56	0.41
1:A:305:LYS:H	1:A:343:ARG:HH12	1.67	0.41
1:B:411:ASN:OD1	1:B:433:ALA:N	2.39	0.41
1:E:261:LYS:HG3	1:E:333:VAL:HG23	2.03	0.41
1:E:399:ILE:H	1:E:399:ILE:HG13	1.68	0.41
1:F:198:PHE:CD2	1:F:240:PHE:HB3	2.56	0.41
1:F:250:LEU:O	1:F:254:MET:HG3	2.21	0.41
1:F:271:GLU:OE2	1:F:320:SER:HB2	2.21	0.41
1:A:299:ALA:HA	1:A:352:LEU:HD13	2.03	0.40
1:B:195:TYR:HE1	1:B:325:ARG:HE	1.69	0.40
1:D:28:SER:HB3	1:D:169:ASN:HD22	1.86	0.40
1:F:25:SER:HB3	1:F:150:ILE:HB	2.03	0.40
1:F:136:ILE:HD11	1:F:242:ILE:HG21	2.02	0.40
1:B:200:GLN:HA	1:B:239:GLY:O	2.22	0.40
1:C:204:ALA:HA	1:C:235:ASN:ND2	2.36	0.40
1:C:376:MET:HB3	1:C:385:VAL:HG11	2.03	0.40
1:C:433:ALA:HA	1:C:446:LEU:HA	2.04	0.40
1:D:236:ILE:HG21	1:F:234:GLY:HA3	2.03	0.40
1:D:242:ILE:HG23	1:D:246:MET:HE2	2.02	0.40
1:D:288:ALA:O	1:D:309:VAL:HA	2.20	0.40
1:D:415:VAL:CG1	1:D:421:LEU:HB2	2.51	0.40
1:F:313:LEU:N	1:F:316:LYS:O	2.47	0.40
1:A:376:MET:HG2	1:A:387:VAL:HG13	2.03	0.40
1:E:421:LEU:HD13	1:E:421:LEU:HA	1.88	0.40
1:A:19:LEU:HD21	1:A:177:VAL:HG11	2.04	0.40
1:D:250:LEU:HD13	1:D:330:THR:OG1	2.21	0.40
1:D:305:LYS:CD	1:D:343:ARG:HH22	2.29	0.40
1:E:385:VAL:O	1:E:385:VAL:HG12	2.21	0.40
1:F:27:VAL:HG21	1:F:115:VAL:HG13	2.04	0.40
1:B:103:ASN:OD1	1:B:211:GLY:N	2.54	0.40
1:B:305:LYS:HB2	1:B:343:ARG:HH12	1.87	0.40
1:D:205:ILE:O	1:D:235:ASN:HB2	2.22	0.40
1:F:214:LEU:O	1:F:222:ILE:HG12	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:TYR:OH	1:A:257:TYR:OH[2_555]	2.05	0.15

## 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	375/440~(85%)	342 (91%)	28 (8%)	5 (1%)	12	48
1	В	388/440 (88%)	358 (92%)	27 (7%)	3 (1%)	19	60
1	С	376/440~(86%)	345 (92%)	29 (8%)	2 (0%)	29	68
1	D	382/440~(87%)	339 (89%)	40 (10%)	3 (1%)	19	60
1	Е	382/440 (87%)	353 (92%)	25 (6%)	4 (1%)	15	54
1	F	373/440~(85%)	352 (94%)	17 (5%)	4 (1%)	14	52
2	G	3/5~(60%)	3 (100%)	0	0	100	100
2	Н	3/5~(60%)	3 (100%)	0	0	100	100
2	Ι	3/5~(60%)	3 (100%)	0	0	100	100
2	J	3/5~(60%)	3 (100%)	0	0	100	100
2	К	3/5~(60%)	3 (100%)	0	0	100	100
2	L	3/5~(60%)	3 (100%)	0	0	100	100
2	М	3/5~(60%)	3 (100%)	0	0	100	100
2	N	3/5~(60%)	3 (100%)	0	0	100	100
2	Ο	3/5~(60%)	3 (100%)	0	0	100	100
2	Р	3/5~(60%)	3 (100%)	0	0	100	100
2	Q	3/5~(60%)	3 (100%)	0	0	100	100
2	R	3/5~(60%)	3 (100%)	0	0	100	100
All	All	2312/2700~(86%)	2125 (92%)	166 (7%)	21 (1%)	17	56



$\operatorname{Mol}$	Chain	$\operatorname{Res}$	Type
1	D	408	ILE
1	F	291	SER
1	F	369	ASN
1	А	335	SER
1	С	436	ILE
1	D	411	ASN
1	Е	383	GLN
1	F	372	GLU
1	В	370	GLY
1	В	409	GLY
1	В	430	SER
1	Е	370	GLY
1	А	175	GLU
1	А	369	ASN
1	D	434	LEU
1	Е	347	GLN
1	Е	407	ILE
1	F	438	ARG
1	А	380	GLY
1	С	408	ILE
1	А	160	VAL

All (21) Ramachandran outliers are listed below:

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	301/350~(86%)	286~(95%)	15~(5%)	24	51
1	В	312/350~(89%)	291~(93%)	21 (7%)	16	43
1	С	302/350~(86%)	293~(97%)	9~(3%)	41	63
1	D	308/350~(88%)	298~(97%)	10 (3%)	39	62
1	Ε	308/350~(88%)	295~(96%)	13 (4%)	30	55
1	F	300/350~(86%)	286~(95%)	14 (5%)	26	53
2	Ι	1/5~(20%)	0	1 (100%)	0	0



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Κ	1/5~(20%)	0	1 (100%)	0
2	М	1/5~(20%)	1 (100%)	0	100 100
All	All	1834/2115~(87%)	1750~(95%)	84 (5%)	27 54

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	19	LEU
1	А	83	LYS
1	А	87	LEU
1	А	124	ASP
1	А	126	LYS
1	А	207	ARG
1	А	281	LYS
1	А	286	ARG
1	А	337	LEU
1	А	343	ARG
1	А	344	ASP
1	А	352	LEU
1	А	379	LYS
1	А	402	LYS
1	А	428	LYS
1	В	15	LEU
1	В	32	GLU
1	В	87	LEU
1	В	96	ASP
1	В	102	THR
1	В	103	ASN
1	В	104	ASN
1	В	121	ARG
1	В	124	ASP
1	В	126	LYS
1	В	133	ARG
1	В	190	LEU
1	В	246	MET
1	В	262	ARG
1	В	280	MET
1	В	312	SER
1	В	320	SER
1	В	422	ARG
1	В	440	ASP



Mol	Chain	Res	Type
1	В	447	MET
1	В	448	GLN
1	С	84	PHE
1	С	103	ASN
1	С	183	SER
1	С	214	LEU
1	С	319	SER
1	С	338	THR
1	С	383	GLN
1	С	402	LYS
1	С	445	LEU
1	D	25	SER
1	D	30	ASN
1	D	34	SER
1	D	82	GLN
1	D	124	ASP
1	D	126	LYS
1	D	190	LEU
1	D	290	VAL
1	D	402	LYS
1	D	435	ASN
1	Е	85	MET
1	Е	156	ASP
1	Е	187	ARG
1	Е	281	LYS
1	Е	291	SER
1	Е	352	LEU
1	Е	401	LEU
1	Е	412	GLN
1	Е	420	GLU
1	Е	423	LYS
1	Е	444	TYR
1	Е	446	LEU
1	Е	447	MET
1	F	85	MET
1	F	87	LEU
1	F	114	LYS
1	F	133	ARG
1	F	148	THR
1	F	265	LEU
1	F	281	LYS
1	F	297	SER



Contr	Continuea front precious page					
Mol	Chain	$\mathbf{Res}$	Type			
1	F	325	ARG			
1	F	336	LYS			
1	F	350	VAL			
1	F	368	PHE			
1	F	377	SER			
1	F	447	MET			
2	Ι	464	LEU			
2	K	464	LEU			

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

Mol	Chain	Res	Type
1	А	355	GLN
1	В	104	ASN
1	С	103	ASN
1	С	169	ASN
1	С	435	ASN
1	D	417	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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	$\langle RSRZ \rangle$	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	381/440~(86%)	-0.35	0 100 100	2,  30,  97,  131	0
1	В	392/440~(89%)	-0.35	1 (0%) 94 90	4,50,117,166	0
1	С	382/440~(86%)	-0.29	3 (0%) 86 79	2, 29, 128, 152	0
1	D	388/440~(88%)	-0.14	7 (1%) 68 59	8, 69, 164, 208	0
1	Ε	388/440~(88%)	-0.21	5 (1%) 77 68	6, 55, 134, 165	0
1	F	379/440~(86%)	-0.35	1 (0%) 94 90	7,35,90,119	0
2	G	5/5~(100%)	-0.30	0 100 100	24,  43,  44,  47	0
2	Н	5/5~(100%)	-0.02	0 100 100	59, 67, 80, 85	0
2	Ι	5/5~(100%)	-0.19	0 100 100	24, 57, 76, 85	0
2	J	5/5~(100%)	-0.12	0 100 100	42, 60, 70, 73	0
2	Κ	5/5~(100%)	-0.11	0 100 100	60, 67, 79, 87	0
2	L	5/5~(100%)	0.24	0 100 100	57, 80, 100, 104	0
2	М	5/5~(100%)	-0.63	0 100 100	26, 33, 59, 59	0
2	Ν	5/5~(100%)	-0.68	0 100 100	54,65,70,72	0
2	Ο	5/5~(100%)	0.28	0 100 100	82, 85, 107, 113	0
2	Р	5/5~(100%)	0.01	0 100 100	50,71,90,98	0
2	Q	5/5~(100%)	-0.20	0 100 100	28, 42, 87, 94	0
2	R	5/5~(100%)	-0.26	0 100 100	61, 65, 79, 90	0
All	All	2370/2700 (87%)	-0.28	17 (0%) 87 82	2, 45, 124, 208	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ε	372	GLU	4.2
1	D	393	GLY	3.6
1	Е	392	THR	3.4



Mol	Chain	Res	Type	RSRZ
1	С	34	SER	3.3
1	D	391	LYS	3.2
1	С	35	THR	2.8
1	В	369	ASN	2.6
1	F	369	ASN	2.5
1	D	388	ASN	2.3
1	Е	390	VAL	2.2
1	Е	369	ASN	2.2
1	Е	391	LYS	2.2
1	D	369	ASN	2.2
1	D	375	GLU	2.2
1	D	392	THR	2.1
1	С	378	ASN	2.1
1	D	370	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.

