

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 08:01 PM JST

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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
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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	Δ	480	2%		
1	A	400	83%	16%	•
1	В	480	2% 7 0%	190/	_
	D	100	7970	10 /0	•
1	С	480		1.60/	
1	U	400	82%	16%	•
1	D	400			
	D	480	82%	16%	•
	_		3%		
1	E	480	83%	15%	·
			2%		
1	F	480	81%	17%	•



Mol	Chain	Length	Quality of chain		
1	G	480	2% 76%	21%	•
1	Н	480	<u>4%</u> 79%	18%	•
1	Ι	480	^{3%} 79%	19%	•
1	J	480	76%	22%	•
1	K	480	71%	26%	•
1	L	480	69%	27%	5%
1	М	480	76%	21%	•
1	N	480	75%	22%	•
1	0	480	68%	30%	•
1	Р	480	66%	29%	•
1	Q	480	76%	22%	•
1	R	480	5%	31%	5%



$7 \mathrm{XDR}$

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 71196 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	Atoms		ZeroOcc	AltConf	Trace			
1	А	480	Total	С	Ν	0	S	0	0	0
		100	3862	2464	639	737	22	Ŭ	0	0
1	В	480	Total	С	Ν	Ο	S	0	0	0
		100	3862	2464	639	737	22	Ŭ		Ŭ
1	C	480	Total	С	Ν	0	S	0	0	0
		100	3862	2464	639	737	22	Ŭ		<u> </u>
1	D	480	Total	С	N	0	S	0	0	0
			3862	2464	639	737	22		_	_
1	Е	479	Total	C	N	0	S	0	0	0
			3854	2459	638	736	21			
1	F	480	Total	C	N	0	S	0	0	0
			3850	2458	633	737	22			
1	G	479	Total	C	N	0	S	0	0	0
			3854	2459	6 <u>38</u>	736	21			
1	Н	480	Total	C DACA	N	0	S	0	0	0
			3862 Tetel	2464	039 N	(3)	22			
1	Ι	480		0		797	3 99	0	0	0
			3802 Tetel	2464	039 N	131	22			
1	J	480		2464	IN 620	797	ວ າາ	0	0	0
			3802 Tatal	2404	039 N	131	<u>ZZ</u>			
1	K	480	10tal 2969	2464	IN 620	0	ວ າາ	0	0	0
			Total	$\frac{2404}{C}$	039 N	151	<u> </u>			
1	L	480	10tai 3862	2464	IN 630	$\frac{0}{737}$	ວ າາ	0	0	0
			Total	2404	039 N	101	22 C			
1	М	480	10tai 3862	2464	1N 630	737	ວ າາ	0	0	0
			Total	2404 C	055 N	0	<u>S</u>			
1	Ν	480	3862	2464	1N 630	737	ນ ງງ	0	0	0
			Total	2404 C	055 N	0	<u>S</u>			
1	Ο	480	3862	2464	639	737	22	0	0	0
			Total	<u> </u>	<u>N</u>	0	S			
1	Р	480	3862	2464	639	737	22	0	0	0
			0002	2101	005	101				

• Molecule 1 is a protein called Glucosylglycerol phosphorylase.



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Q	480	Total 3862	C 2464	N 639	0 737	S 22	0	0	0
1	R	480	Total 3862	C 2464	N 639	0 737	S 22	0	0	0

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	163	Total O 163 163	0	0
2	В	132	Total O 132 132	0	0
2	С	148	Total O 148 148	0	0
2	D	93	Total O 93 93	0	0
2	Е	146	Total O 146 146	0	0
2	F	90	Total O 90 90	0	0
2	G	104	Total O 104 104	0	0
2	Н	117	Total O 117 117	0	0
2	Ι	83	Total O 83 83	0	0
2	J	80	Total O 80 80	0	0
2	К	101	Total O 101 101	0	0
2	L	67	Total O 67 67	0	0
2	М	74	Total O 74 74	0	0
2	Ν	94	Total O 94 94	0	0
2	Ο	46	$\begin{array}{cc} \text{Total} & \text{O} \\ 46 & 46 \end{array}$	0	0
2	Р	46	Total O 46 46	0	0
2	Q	56	$\begin{array}{cc} \text{Total} & \text{O} \\ 56 & 56 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	68	Total O 68 68	0	0



3 Residue-property plots (i)

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

L414 • Molecule 1: Glucosylglycerol phosphorylase 2% Chain D: 82% 16% E CI 1395 1395 1396 1396 • Molecule 1: Glucosylglycerol phosphorylase Chain E: 83% 15% • Molecule 1: Glucosylglycerol phosphorylase Chain F: 81% 17% • Molecule 1: Glucosylglycerol phosphorylase 2% Chain G: 76% 21%





• Molecule 1: Glucosylglycerol phosphorylase



IL458 A325 IL458 A325 K4461 333 F460 A325 K4461 333 F460 A325 F460 A325 F461 333 E471 S333 E479 A333 E479 B365 E386 B365 B391 L393 B393 B406 B406 B430</

• Molecule 1: Glucosylglycerol phosphorylase



• Molecule 1: Glucosylglycerol phosphorylase









 \bullet Molecule 1: Glucosylglycerol phosphorylase





• Molecule 1: Glucosylglycerol phosphorylase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	102.27Å 185.17 Å 257.62 Å	Deperitor
a, b, c, α , β , γ	90.00° 101.56° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	33.40 - 2.40	Depositor
Resolution (A)	49.22 - 2.40	EDS
% Data completeness	99.8 (33.40-2.40)	Depositor
(in resolution range)	95.3 (49.22-2.40)	EDS
R_{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.69 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.194 , 0.237	Depositor
Π, Π_{free}	0.205 , 0.242	DCC
R_{free} test set	18044 reflections (4.99%)	wwPDB-VP
Wilson B-factor $(Å^2)$	39.6	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 44.1	EDS
L-test for twinning ²	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	71196	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.50	0/3959	0.67	0/5384	
1	В	0.48	0/3959	0.65	0/5384	
1	С	0.50	0/3959	0.66	0/5384	
1	D	0.48	0/3959	0.65	0/5384	
1	Ε	0.49	0/3951	0.65	0/5374	
1	F	0.48	0/3947	0.64	0/5370	
1	G	0.50	0/3951	0.66	0/5374	
1	Н	0.50	0/3959	0.66	0/5384	
1	Ι	0.47	0/3959	0.64	0/5384	
1	J	0.48	0/3959	0.63	0/5384	
1	Κ	0.52	0/3959	0.63	0/5384	
1	L	0.48	0/3959	0.63	0/5384	
1	М	0.47	0/3959	0.62	0/5384	
1	Ν	0.48	0/3959	0.65	0/5384	
1	0	0.46	0/3959	0.60	0/5384	
1	Р	0.47	0/3959	0.61	0/5384	
1	Q	0.45	0/3959	0.63	0/5384	
1	R	0.50	0/3959	0.62	0/5384	
All	All	0.48	0/71234	0.64	0/96878	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3862	0	3724	48	0
1	В	3862	0	3724	63	0
1	С	3862	0	3724	53	0
1	D	3862	0	3724	50	0
1	Е	3854	0	3712	49	0
1	F	3850	0	3702	56	0
1	G	3854	0	3712	63	0
1	Н	3862	0	3724	57	0
1	Ι	3862	0	3724	62	0
1	J	3862	0	3724	53	0
1	Κ	3862	0	3724	83	0
1	L	3862	0	3724	86	0
1	М	3862	0	3724	56	0
1	Ν	3862	0	3724	66	0
1	0	3862	0	3724	93	0
1	Р	3862	0	3724	100	0
1	Q	3862	0	3724	68	0
1	R	3862	0	3724	116	0
2	А	163	0	0	2	0
2	В	132	0	0	2	0
2	С	148	0	0	5	0
2	D	93	0	0	2	0
2	Е	146	0	0	6	0
2	F	90	0	0	3	0
2	G	104	0	0	5	0
2	Н	117	0	0	3	0
2	Ι	83	0	0	2	0
2	J	80	0	0	1	0
2	Κ	101	0	0	3	0
2	L	67	0	0	3	0
2	М	74	0	0	1	0
2	N	94	0	0	0	0
2	0	46	0	0	2	0
2	Р	46	0	0	3	0
2	Q	56	0	0	2	0
2	R	68	0	0	2	0
All	All	71196	0	66986	1185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1185) 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:R:464:LYS:HE2	1:R:466:THR:HG23	1.48	0.95
1:F:329:HIS:HA	1:F:334:ILE:HD11	1.50	0.92
1:M:66:THR:HG22	1:M:68:ASP:H	1.34	0.91
1:Q:472:THR:HG23	1:Q:474:GLU:H	1.38	0.89
1:J:12:TYR:HB2	1:J:15:ARG:HB2	1.54	0.89
1:P:287:THR:HG22	1:P:289:ASP:H	1.38	0.86
1:K:306:LYS:HD3	1:K:331:VAL:HG23	1.57	0.86
1:E:101:ASN:O	1:E:104:ASP:HB2	1.76	0.85
1:E:377:CYS:SG	2:E:575:HOH:O	2.34	0.85
1:C:472:THR:HG23	1:C:474:GLU:H	1.43	0.83
1:P:33:GLU:HB3	1:P:419:LYS:HD3	1.61	0.82
1:R:177:GLY:HA2	1:R:224:HIS:HD2	1.42	0.82
1:I:10:ILE:HG23	1:I:369:TYR:HA	1.59	0.81
1:P:78:ASP:HA	1:P:185:ASN:HD21	1.43	0.81
1:I:239:GLN:HG3	1:I:249:PRO:HB2	1.63	0.80
1:R:469:ASP:HB2	1:R:476:ARG:HD2	1.64	0.78
1:E:460:PHE:HA	1:K:133:GLU:O	1.83	0.78
1:F:479:GLU:OE1	1:F:479:GLU:N	2.17	0.77
1:F:211:TYR:O	1:F:215:ASP:HB2	1.84	0.77
1:I:371:VAL:HG21	1:I:393:ASN:O	1.83	0.77
1:J:47:ASN:HD22	1:J:91:GLU:HG3	1.47	0.77
1:B:327:ASN:HB2	1:R:307:VAL:HB	1.67	0.77
1:I:450:TYR:HE1	1:I:470:VAL:HG13	1.49	0.77
1:C:12:TYR:HB2	1:C:15:ARG:HB2	1.67	0.76
1:P:391:ASP:HA	1:P:394:ARG:HB2	1.67	0.76
1:H:47:ASN:HD22	1:H:91:GLU:HG3	1.51	0.76
1:B:328:ILE:HD12	1:B:328:ILE:H	1.50	0.75
1:N:12:TYR:HB2	1:N:15:ARG:HB2	1.69	0.75
1:H:378:ASN:HB3	1:H:392:ILE:HD13	1.70	0.74
1:I:306:LYS:HE3	1:I:329:HIS:HB3	1.70	0.74
1:P:303:GLU:HA	1:P:306:LYS:HD3	1.70	0.73
1:F:469:ASP:OD1	1:F:471:GLU:HB2	1.89	0.73
1:M:30:HIS:CD2	1:M:406:ILE:HG13	2.24	0.73
1:K:33:GLU:HB3	1:K:419:LYS:HG2	1.71	0.73
1:O:172:MET:HE3	1:O:172:MET:HA	1.71	0.73
1:H:12:TYR:HB2	1:H:15:ARG:HB2	1.72	0.72
1:Q:130:ILE:HD13	1:Q:136:PRO:HG3	1.71	0.72
1:H:11:CYS:SG	1:H:38:LEU:HD21	2.30	0.72
1:I:301:PRO:HD2	1:I:304:LYS:HG3	1.70	0.72
1:B:120:ILE:HG21	1:B:125:MET:HE2	1.72	0.72
1:N:371:VAL:HG21	1:N:393:ASN:O	1.90	0.72
1:O:10:ILE:HG23	1:O:369:TYR:HA	1.71	0.72

 $7 \mathrm{XDR}$



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:142:LEU:HD12	1:B:146:THR:HB	1.71	0.71
1:Q:469:ASP:HB3	1:Q:472:THR:HG22	1.71	0.71
1:J:449:ASP:HB3	1:J:470:VAL:HG22	1.71	0.71
1:N:82:ASP:OD2	1:N:188:ARG:NH1	2.23	0.71
1:H:324:SER:OG	1:H:325:ALA:N	2.19	0.70
1:I:120:ILE:HG21	1:I:125:MET:HE2	1.73	0.70
1:N:450:TYR:HE1	1:N:470:VAL:HG13	1.56	0.70
1:A:400:GLU:HG3	1:A:404:GLN:HE22	1.57	0.70
1:C:241:ALA:O	1:C:245:ARG:HG2	1.92	0.70
1:G:314:ALA:HB2	2:G:505:HOH:O	1.91	0.70
1:L:391:ASP:HA	1:L:394:ARG:HB2	1.74	0.70
1:J:459:ASN:HB3	1:O:323:ARG:HH21	1.56	0.69
1:K:460:PHE:HE1	1:L:130:ILE:HD11	1.58	0.69
1:D:12:TYR:HB2	1:D:15:ARG:HB2	1.73	0.69
1:N:127:LYS:NZ	1:N:200:GLY:O	2.24	0.69
1:L:414:LEU:O	1:L:418:MET:HG3	1.92	0.69
1:I:114:VAL:HG21	1:I:137:PHE:HB3	1.74	0.69
1:J:144:ASP:OD1	1:J:146:THR:HG22	1.92	0.69
1:F:9:LEU:HD23	1:F:38:LEU:HD11	1.75	0.69
1:H:249:PRO:HD2	1:H:280:ASN:O	1.93	0.69
1:P:67:TRP:CZ3	1:P:182:LYS:HG3	2.29	0.68
1:M:405:ASP:HA	1:M:408:LYS:HD3	1.75	0.68
1:P:447:HIS:ND1	2:P:502:HOH:O	2.26	0.68
1:H:245:ARG:HG3	1:H:245:ARG:HH11	1.59	0.68
1:A:38:LEU:CD2	1:A:40:ILE:HG12	2.24	0.67
1:E:15:ARG:HD2	1:E:396:TYR:CE2	2.29	0.67
1:G:12:TYR:HB2	1:G:15:ARG:HG2	1.74	0.67
1:E:244:ARG:HG2	1:E:244:ARG:HH11	1.59	0.67
1:G:400:GLU:HG3	1:L:409:PRO:HG2	1.76	0.67
1:L:380:HIS:O	1:L:384:GLU:HG2	1.95	0.67
1:R:46:SER:HB3	1:R:51:GLY:HA2	1.77	0.67
1:D:21:LYS:HE3	1:D:69:ASP:OD1	1.96	0.66
1:H:279:ARG:HG2	1:H:280:ASN:N	2.10	0.66
1:P:12:TYR:HB2	1:P:15:ARG:HB2	1.75	0.66
1:L:110:LEU:HD11	1:L:161:LEU:HD22	1.78	0.66
1:M:30:HIS:HD2	1:M:406:ILE:HG13	1.60	0.66
1:R:15:ARG:HG3	1:R:370:TYR:OH	1.96	0.66
1:N:252:PHE:O	1:N:255:PRO:HD2	1.95	0.66
1:B:132:LYS:HE3	1:B:136:PRO:HA	1.78	0.66
1:I:450:TYR:CE1	1:I:470:VAL:HG13	2.30	0.66
1:I:309:ILE:HG21	1:I:334:ILE:HD12	1.77	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:47:ASN:HD22	1:B:91:GLU:HG3	1.62	0.65
1:F:12:TYR:HB2	1:F:15:ARG:HB2	1.77	0.65
1:R:464:LYS:HE2	1:R:466:THR:CG2	2.23	0.65
1:O:141:THR:HG22	1:O:147:LYS:HG2	1.77	0.65
1:O:382:LEU:HD11	1:O:396:TYR:HD1	1.61	0.65
1:A:38:LEU:HD23	1:A:40:ILE:HG12	1.78	0.65
1:D:124:ASP:HA	1:D:127:LYS:HD2	1.79	0.65
1:C:9:LEU:HD23	1:C:38:LEU:HD11	1.79	0.65
1:K:10:ILE:HD11	1:K:367:GLN:HB3	1.78	0.64
1:G:142:LEU:HD12	1:G:146:THR:HB	1.79	0.64
1:L:131:ARG:CZ	1:L:131:ARG:H	2.09	0.64
1:Q:53:SER:HB2	1:Q:158:GLN:HG3	1.78	0.64
1:D:405:ASP:HA	1:D:408:LYS:HD3	1.80	0.64
1:I:389:LEU:O	1:I:392:ILE:HG22	1.97	0.64
1:O:378:ASN:HB3	1:O:392:ILE:HD11	1.78	0.64
1:R:76:LYS:HD3	1:R:77:TYR:CE1	2.32	0.64
1:Q:252:PHE:O	1:Q:255:PRO:HD2	1.97	0.64
1:A:10:ILE:HG12	1:A:369:TYR:HD1	1.63	0.64
1:L:14:ASP:OD1	1:L:14:ASP:N	2.30	0.63
1:R:20:LEU:HD12	1:R:65:GLY:HA3	1.80	0.63
1:O:398:THR:OG1	1:O:400:GLU:HG2	1.98	0.63
1:0:419:LYS:O	1:O:423:ASN:ND2	2.28	0.63
1:E:3:LEU:HD11	1:E:186:LEU:HD13	1.81	0.63
1:L:66:THR:HG23	1:L:68:ASP:H	1.64	0.63
1:R:11:CYS:SG	1:R:38:LEU:HD21	2.38	0.63
1:R:12:TYR:HB2	1:R:15:ARG:HB2	1.79	0.63
1:F:383:MET:HE1	1:F:389:LEU:HD23	1.79	0.63
1:A:460:PHE:HE1	1:C:130:ILE:HD11	1.64	0.63
1:N:141:THR:OG1	1:N:147:LYS:NZ	2.30	0.63
1:C:469:ASP:HB3	1:C:472:THR:HG22	1.81	0.63
1:A:240:TYR:CZ	1:A:278:PRO:HD3	2.35	0.62
1:O:466:THR:HG23	1:O:475:THR:HG23	1.80	0.62
1:R:12:TYR:HB2	1:R:15:ARG:HG2	1.80	0.62
1:R:405:ASP:HA	1:R:408:LYS:HD3	1.80	0.62
1:B:286:ASP:OD1	1:B:286:ASP:N	2.29	0.62
1:D:63:LYS:HD3	1:O:63:LYS:HE2	1.81	0.62
1:K:47:ASN:ND2	1:K:89:SER:OG	2.25	0.62
1:O:142:LEU:HD12	1:O:146:THR:HB	1.80	0.62
1:L:97:ASP:HB3	1:L:107:TYR:HD2	1.65	0.62
1:R:21:LYS:O	1:R:25:THR:HG23	2.00	0.62
1:L:292:CYS:SG	1:L:294:PRO:HD2	2.39	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:378:ASN:HB3	1:B:392:ILE:HD11	1.82	0.61
1:L:316:SER:HB2	1:L:339:CYS:HB3	1.82	0.61
1:N:138:ARG:HE	1:N:140:VAL:HG12	1.63	0.61
1:K:258:LEU:HD12	1:K:285:LEU:HD11	1.81	0.61
1:P:382:LEU:HD11	1:P:396:TYR:HD1	1.65	0.61
1:L:325:ALA:HB1	1:L:333:ALA:HA	1.83	0.61
1:G:313:ASP:OD2	1:G:314:ALA:N	2.34	0.61
1:E:323:ARG:NH2	2:E:506:HOH:O	2.32	0.61
1:F:33:GLU:OE2	1:F:419:LYS:NZ	2.26	0.61
1:F:460:PHE:HE1	1:J:130:ILE:HD11	1.66	0.61
1:K:309:ILE:HG21	1:K:334:ILE:HD13	1.82	0.61
1:P:31:LEU:HD21	1:P:373:LEU:HD21	1.83	0.61
1:I:131:ARG:O	1:I:323:ARG:HB3	2.00	0.61
1:O:209:GLU:OE2	1:O:209:GLU:N	2.28	0.61
1:P:244:ARG:HA	1:P:279:ARG:HH22	1.66	0.61
1:P:322:ARG:NH1	1:P:332:GLY:O	2.33	0.61
1:B:389:LEU:O	1:B:392:ILE:HG22	2.01	0.61
1:H:38:LEU:HD22	1:H:40:ILE:HG13	1.82	0.60
1:I:15:ARG:HG2	1:I:370:TYR:OH	2.00	0.60
1:D:192:PHE:CE1	1:D:232:VAL:HG22	2.35	0.60
1:P:338:THR:HG21	1:P:389:LEU:HB3	1.81	0.60
1:R:177:GLY:HA2	1:R:224:HIS:CD2	2.32	0.60
1:E:12:TYR:HB2	1:E:15:ARG:HB2	1.81	0.60
1:R:303:GLU:O	1:R:307:VAL:HG13	2.02	0.60
1:J:47:ASN:ND2	1:J:91:GLU:HG3	2.15	0.60
1:C:472:THR:HG23	1:C:474:GLU:N	2.12	0.60
1:H:405:ASP:HA	1:H:408:LYS:HD3	1.83	0.60
1:N:102:GLY:HA2	1:N:142:LEU:HD22	1.82	0.60
1:L:47:ASN:ND2	1:L:89:SER:OG	2.35	0.60
1:I:12:TYR:HB2	1:I:15:ARG:HB2	1.84	0.59
1:M:338:THR:HG21	1:M:389:LEU:HB3	1.83	0.59
1:P:110:LEU:HD11	1:P:161:LEU:HD22	1.84	0.59
1:J:457:ASP:HB3	1:J:462:THR:HG22	1.84	0.59
1:N:414:LEU:O	1:N:418:MET:HG3	2.03	0.59
1:D:15:ARG:HD2	1:D:396:TYR:CE2	2.37	0.59
1:D:47:ASN:HD22	1:D:91:GLU:HG3	1.68	0.59
1:K:286:ASP:OD1	1:K:356:ARG:NH2	2.35	0.59
1:I:472:THR:OG1	1:I:474:GLU:HG2	2.03	0.59
1:M:240:TYR:O	1:M:244:ARG:HD3	2.03	0.59
1:E:459:ASN:HB3	1:K:323:ARG:HH11	1.66	0.59
1:J:220:VAL:HA	1:J:223:LYS:HE2	1.85	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:27:VAL:HA	1:M:31:LEU:HD12	1.84	0.59
1:A:138:ARG:NE	2:A:509:HOH:O	2.35	0.59
1:F:9:LEU:HB3	1:F:38:LEU:HD12	1.83	0.59
1:J:303:GLU:O	1:J:307:VAL:HG13	2.02	0.59
1:P:78:ASP:HA	1:P:185:ASN:ND2	2.17	0.59
1:K:142:LEU:HB2	1:K:144:ASP:OD1	2.03	0.58
1:K:316:SER:HB2	1:K:339:CYS:HB3	1.85	0.58
1:O:252:PHE:O	1:O:255:PRO:HD2	2.03	0.58
1:I:152:CYS:SG	1:I:155:THR:O	2.61	0.58
1:N:80:CYS:HB2	1:N:186:LEU:HB3	1.85	0.58
1:C:257:LEU:HD21	1:C:270:LEU:HA	1.85	0.58
1:K:79:LEU:HD23	1:K:184:VAL:HG12	1.85	0.58
1:D:47:ASN:ND2	1:D:91:GLU:HG3	2.19	0.58
1:J:152:CYS:HB2	1:J:158:GLN:O	2.04	0.58
1:A:12:TYR:HB2	1:A:15:ARG:HB2	1.85	0.58
1:C:113:HIS:ND1	2:C:504:HOH:O	2.32	0.58
1:I:249:PRO:HD2	1:I:280:ASN:O	2.04	0.58
1:K:328:ILE:O	1:K:334:ILE:HD11	2.03	0.58
1:E:101:ASN:HB2	1:E:105:SER:HB2	1.86	0.58
1:L:195:THR:HA	2:L:502:HOH:O	2.03	0.58
1:B:303:GLU:HA	1:B:306:LYS:HD2	1.85	0.58
1:L:325:ALA:HB1	1:L:333:ALA:CB	2.34	0.58
1:A:257:LEU:HD21	1:A:270:LEU:HA	1.86	0.58
1:M:12:TYR:HB2	1:M:15:ARG:HB2	1.85	0.58
1:E:460:PHE:HE1	1:K:130:ILE:HD11	1.68	0.57
1:C:318:ASP:O	1:C:338:THR:OG1	2.22	0.57
1:M:152:CYS:HB2	1:M:158:GLN:O	2.04	0.57
1:M:205:LEU:HD21	1:M:232:VAL:HG11	1.86	0.57
1:N:13:PRO:HB3	1:N:20:LEU:HD21	1.86	0.57
1:O:9:LEU:HD23	1:O:38:LEU:HD11	1.86	0.57
1:O:188:ARG:NH1	1:0:190:ASP:OD1	2.37	0.57
1:R:279:ARG:HH11	1:R:280:ASN:HD21	1.50	0.57
1:F:319:PRO:HG2	1:F:321:MET:CE	2.35	0.57
1:Q:353:ILE:HG23	1:Q:417:LEU:HD11	1.85	0.57
1:P:125:MET:HA	1:P:128:ILE:HD12	1.86	0.57
1:Q:472:THR:HG23	1:Q:474:GLU:N	2.15	0.57
1:G:467:TYR:CZ	1:G:476:ARG:HB2	2.40	0.57
1:L:57:HIS:HB2	1:L:175:TYR:CD1	2.40	0.57
1:L:323:ARG:HD3	1:L:324:SER:H	1.69	0.57
1:M:378:ASN:HB3	1:M:392:ILE:HG23	1.86	0.57
1:0:12:TYR:HB2	1:0:15:ARG:HB2	1.87	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:141:THR:CG2	1:M:147:LYS:HE2	2.34	0.57
1:N:405:ASP:HA	1:N:408:LYS:HD3	1.85	0.57
1:K:252:PHE:O	1:K:255:PRO:HD2	2.04	0.57
1:R:24:TYR:OH	1:R:76:LYS:HD2	2.03	0.57
1:R:40:ILE:HB	1:R:43:PHE:HE2	1.70	0.57
1:I:312:ILE:HG21	1:I:337:LEU:HD13	1.87	0.57
1:F:166:ASP:O	1:F:170:GLN:HG3	2.05	0.56
1:L:219:GLN:O	1:L:223:LYS:HG2	2.05	0.56
1:O:53:SER:HB2	1:O:158:GLN:HG3	1.87	0.56
1:C:33:GLU:HB2	1:C:419:LYS:HD3	1.87	0.56
1:H:140:VAL:HG22	1:H:148:THR:HG22	1.86	0.56
1:L:12:TYR:HB2	1:L:15:ARG:HG2	1.85	0.56
1:P:402:VAL:O	1:P:406:ILE:HG12	2.04	0.56
1:Q:131:ARG:HB2	1:Q:131:ARG:CZ	2.35	0.56
1:R:286:ASP:OD1	1:R:286:ASP:N	2.37	0.56
1:G:179:LEU:O	1:G:184:VAL:HG13	2.06	0.56
1:P:286:ASP:OD1	1:P:286:ASP:N	2.30	0.56
1:L:398:THR:HG23	1:L:401:GLU:HB2	1.87	0.56
1:M:472:THR:HG22	1:M:474:GLU:HB3	1.87	0.56
1:P:131:ARG:O	1:P:323:ARG:HB2	2.06	0.56
1:Q:405:ASP:HA	1:Q:408:LYS:HD3	1.87	0.56
1:D:192:PHE:HE1	1:D:232:VAL:HG22	1.70	0.56
1:E:265:ALA:CB	1:K:324:SER:HB2	2.36	0.56
1:F:303:GLU:HG3	1:F:304:LYS:N	2.21	0.56
1:G:152:CYS:HB2	1:G:158:GLN:O	2.06	0.56
1:0:249:PRO:HD2	1:O:281:MET:HA	1.87	0.56
1:D:58:LYS:HG2	1:D:178:PHE:CG	2.40	0.56
1:N:382:LEU:HD23	1:N:391:ASP:HB3	1.88	0.56
1:C:467:TYR:CE2	1:C:476:ARG:HG3	2.41	0.56
1:B:478:LEU:HD13	1:B:480:CYS:H	1.70	0.56
1:P:257:LEU:HD21	1:P:270:LEU:HA	1.87	0.56
1:L:61:ASP:O	1:L:64:VAL:HG22	2.06	0.56
1:G:476:ARG:CZ	1:G:476:ARG:HB3	2.35	0.55
1:H:43:PHE:HB2	1:H:64:VAL:HG21	1.87	0.55
1:H:450:TYR:HE1	1:H:470:VAL:HB	1.71	0.55
1:R:53:SER:HB2	1:R:158:GLN:HG3	1.87	0.55
1:K:57:HIS:HB2	1:K:175:TYR:CD1	2.40	0.55
1:P:414:LEU:O	1:P:418:MET:HG3	2.06	0.55
1:Q:219:GLN:O	1:Q:223:LYS:HD2	2.06	0.55
1:R:15:ARG:HG3	1:R:370:TYR:CZ	2.41	0.55
1:A:229:LEU:HD21	1:A:250:TYR:CZ	2.41	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:382:LEU:O	1:F:385:GLN:HG3	2.06	0.55
1:O:178:PHE:O	1:O:182:LYS:HG2	2.07	0.55
1:P:249:PRO:HD2	1:P:281:MET:HA	1.87	0.55
1:K:12:TYR:HB2	1:K:15:ARG:HB2	1.89	0.55
1:B:252:PHE:O	1:B:255:PRO:HD2	2.06	0.55
1:G:340:THR:OG1	1:G:343:ASP:HB2	2.07	0.55
1:N:128:ILE:HG22	1:N:130:ILE:HG12	1.89	0.55
1:K:431:PHE:HB2	1:K:445:TRP:CH2	2.41	0.55
1:P:294:PRO:HG3	1:P:322:ARG:NH2	2.22	0.55
1:Q:125:MET:HA	1:Q:128:ILE:HD12	1.87	0.55
1:Q:381:GLU:HG2	1:Q:385:GLN:HE21	1.71	0.55
1:B:47:ASN:ND2	1:B:91:GLU:HG3	2.21	0.55
1:A:152:CYS:HB2	1:A:158:GLN:O	2.06	0.55
1:C:229:LEU:HD21	1:C:250:TYR:CZ	2.41	0.55
1:D:391:ASP:HA	1:D:394:ARG:HB2	1.89	0.55
1:G:116:LYS:HG2	1:G:117:PHE:N	2.21	0.55
1:H:90:ASP:HB3	1:H:159:ILE:HD11	1.89	0.55
1:R:94:GLU:HA	1:R:107:TYR:CD1	2.42	0.55
1:I:155:THR:HG22	1:I:156:GLU:H	1.71	0.55
1:O:382:LEU:HD11	1:O:396:TYR:CD1	2.42	0.55
1:I:378:ASN:HB3	1:I:392:ILE:HG13	1.88	0.55
1:K:19:ASN:ND2	2:K:504:HOH:O	2.35	0.55
1:L:9:LEU:HD23	1:L:38:LEU:HD21	1.89	0.55
1:O:180:THR:HG21	1:O:224:HIS:HB3	1.88	0.54
1:O:306:LYS:HE2	1:O:331:VAL:HG13	1.89	0.54
1:B:120:ILE:CG2	1:B:125:MET:HE2	2.37	0.54
1:J:24:TYR:OH	1:J:76:LYS:HD3	2.07	0.54
1:0:286:ASP:OD1	1:O:286:ASP:N	2.40	0.54
1:F:195:THR:HA	2:F:504:HOH:O	2.08	0.54
1:G:205:LEU:HD21	1:G:232:VAL:HG11	1.89	0.54
1:J:142:LEU:HD12	1:J:146:THR:HG23	1.89	0.54
1:K:200:GLY:N	2:K:506:HOH:O	2.39	0.54
1:K:327:ASN:HB3	1:K:330:SER:HB3	1.88	0.54
1:P:82:ASP:OD2	1:P:188:ARG:NH1	2.40	0.54
1:A:252:PHE:O	1:A:255:PRO:HD2	2.07	0.54
1:E:400:GLU:O	1:E:404:GLN:HG3	2.08	0.54
1:Q:469:ASP:HB3	1:Q:472:THR:CG2	2.37	0.54
1:K:249:PRO:HD2	1:K:281:MET:HA	1.89	0.54
1:O:94:GLU:HA	1:O:107:TYR:CD2	2.43	0.54
1:P:103:PHE:HE1	1:P:113:HIS:CE1	2.26	0.54
1:P:132:LYS:H	1:P:132:LYS:HD2	1.72	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:245:ARG:HH11	1:H:245:ARG:CG	2.21	0.54
1:H:469:ASP:HB2	1:H:476:ARG:HD2	1.90	0.54
1:J:26:VAL:HG13	1:J:30:HIS:HD2	1.73	0.54
1:L:219:GLN:HE22	1:L:223:LYS:HZ2	1.56	0.54
1:P:382:LEU:HA	1:P:385:GLN:HE22	1.72	0.54
1:G:114:VAL:HG21	1:G:137:PHE:HB3	1.88	0.54
1:N:306:LYS:HE3	1:N:329:HIS:HB3	1.89	0.54
1:C:460:PHE:HE1	1:D:130:ILE:HD11	1.73	0.53
1:I:31:LEU:HB3	1:I:35:ILE:HG12	1.90	0.53
1:I:286:ASP:HB3	1:I:341:PHE:HB2	1.89	0.53
1:J:414:LEU:O	1:J:418:MET:HG3	2.08	0.53
1:K:263:LEU:O	1:L:324:SER:HB3	2.07	0.53
1:I:452:CYS:HA	1:I:466:THR:O	2.09	0.53
1:O:441:VAL:HG13	1:O:456:VAL:HB	1.90	0.53
1:R:38:LEU:CD2	1:R:40:ILE:HG12	2.39	0.53
1:R:61:ASP:HB3	1:R:64:VAL:HG13	1.90	0.53
1:C:423:ASN:ND2	2:C:518:HOH:O	2.40	0.53
1:J:76:LYS:HE3	1:J:77:TYR:CE2	2.44	0.53
1:N:138:ARG:NE	1:N:140:VAL:HG12	2.22	0.53
1:P:141:THR:HG23	1:P:145:GLY:HA2	1.89	0.53
1:C:237:SER:HB2	1:R:275:ARG:HB3	1.89	0.53
1:H:61:ASP:HB3	1:H:64:VAL:HG13	1.89	0.53
1:K:286:ASP:HB3	1:K:341:PHE:HB2	1.91	0.53
1:0:15:ARG:HD2	1:O:396:TYR:CE2	2.44	0.53
1:A:474:GLU:HG3	1:A:476:ARG:HD3	1.90	0.53
1:D:378:ASN:HB3	1:D:392:ILE:HG12	1.89	0.53
1:F:378:ASN:HB3	1:F:392:ILE:HD11	1.90	0.53
1:C:414:LEU:O	1:C:418:MET:HG3	2.08	0.53
1:D:281:MET:O	1:D:364:GLY:HA3	2.09	0.53
1:N:67:TRP:O	1:N:71:GLU:HG2	2.08	0.53
1:O:230:PRO:HG2	1:O:247:MET:HE3	1.90	0.53
1:P:378:ASN:OD1	1:P:378:ASN:N	2.41	0.53
1:R:87:HIS:CD2	1:R:158:GLN:HG2	2.44	0.53
1:I:80:CYS:HB2	1:I:186:LEU:HB3	1.91	0.53
1:P:96:THR:O	1:P:99:ILE:HG22	2.09	0.53
1:R:327:ASN:O	1:R:328:ILE:HG12	2.08	0.53
1:R:414:LEU:O	1:R:418:MET:HG3	2.08	0.53
1:G:252:PHE:O	1:G:255:PRO:HD2	2.08	0.53
1:F:229:LEU:HD21	1:F:250:TYR:CZ	2.45	0.52
1:N:280:ASN:N	1:N:280:ASN:OD1	2.38	0.52
1:R:74:THR:HG21	1:R:183:GLY:HA3	1.92	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:15:ARG:HG2	1:K:370:TYR:OH	2.08	0.52
1:G:101:ASN:HB2	1:G:105:SER:HB2	1.91	0.52
1:K:242:ILE:HG23	1:K:247:MET:HB2	1.90	0.52
1:K:21:LYS:HE2	1:K:69:ASP:OD1	2.09	0.52
1:N:113:HIS:O	1:N:116:LYS:HG2	2.09	0.52
1:R:308:LEU:O	1:R:312:ILE:HG12	2.10	0.52
1:R:316:SER:HB2	1:R:339:CYS:HB2	1.90	0.52
1:E:140:VAL:HG12	1:E:148:THR:HG23	1.91	0.52
1:J:402:VAL:O	1:J:406:ILE:HG12	2.10	0.52
1:M:151:TRP:CD2	1:M:197:LYS:HD3	2.44	0.52
1:M:229:LEU:HD21	1:M:250:TYR:CZ	2.45	0.52
1:Q:128:ILE:HG22	1:Q:130:ILE:HG12	1.91	0.52
1:Q:130:ILE:HG13	1:Q:323:ARG:HH21	1.74	0.52
1:Q:400:GLU:O	1:Q:404:GLN:HG2	2.09	0.52
1:R:61:ASP:OD1	1:R:62:PRO:HD2	2.10	0.52
1:P:14:ASP:OD1	1:P:14:ASP:N	2.43	0.52
1:A:460:PHE:CE1	1:C:130:ILE:HD11	2.44	0.52
1:C:9:LEU:HB3	1:C:38:LEU:HD12	1.90	0.52
1:L:252:PHE:O	1:L:255:PRO:HD2	2.09	0.52
1:R:88:ILE:HG23	1:R:161:LEU:HD21	1.92	0.52
1:A:249:PRO:HD2	1:A:281:MET:HA	1.91	0.52
1:A:323:ARG:HH21	1:D:459:ASN:HB3	1.74	0.52
1:B:249:PRO:HG2	1:B:281:MET:HB3	1.90	0.52
1:J:10:ILE:HD11	1:J:367:GLN:HB3	1.90	0.52
1:J:27:VAL:HG22	1:J:31:LEU:HD12	1.92	0.52
1:K:286:ASP:OD1	1:K:286:ASP:N	2.43	0.52
1:C:130:ILE:HD13	1:C:136:PRO:HG3	1.91	0.52
1:G:12:TYR:CB	1:G:15:ARG:HG2	2.39	0.52
1:K:138:ARG:HH11	1:K:159:ILE:HD11	1.73	0.52
1:O:258:LEU:HD12	1:O:285:LEU:HD21	1.91	0.52
1:Q:12:TYR:HB2	1:Q:15:ARG:HG2	1.91	0.52
1:Q:207:GLU:HG2	1:Q:211:TYR:CE2	2.44	0.52
1:R:398:THR:OG1	1:R:400:GLU:HG2	2.10	0.52
1:R:455:PHE:HB3	1:R:464:LYS:CG	2.40	0.52
1:D:130:ILE:HD12	1:D:130:ILE:O	2.10	0.52
1:F:80:CYS:HB2	1:F:186:LEU:HB3	1.91	0.52
1:G:328:ILE:HG13	1:G:329:HIS:CE1	2.45	0.52
1:I:10:ILE:HD12	1:I:39:HIS:CD2	2.46	0.52
1:J:252:PHE:O	1:J:255:PRO:HD2	2.09	0.52
1:P:2:LEU:HD21	1:P:185:ASN:O	2.10	0.52
1:G:9:LEU:HB3	1:G:38:LEU:CD2	2.40	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:245:ARG:O	1:I:246:ASN:HB2	2.10	0.51
1:L:325:ALA:HB1	1:L:333:ALA:CA	2.40	0.51
1:L:431:PHE:HE1	1:L:443:MET:HB3	1.74	0.51
1:M:254:LEU:HD11	1:M:258:LEU:HD22	1.92	0.51
1:D:2:LEU:HD12	1:D:3:LEU:HG	1.91	0.51
1:F:469:ASP:OD2	1:F:476:ARG:NH1	2.42	0.51
1:N:53:SER:HB2	1:N:158:GLN:HG3	1.91	0.51
1:O:316:SER:HB2	1:O:339:CYS:HB2	1.93	0.51
1:P:10:ILE:HD11	1:P:367:GLN:OE1	2.10	0.51
1:E:81:VAL:HG22	1:E:184:VAL:HG11	1.93	0.51
1:F:286:ASP:OD1	1:F:286:ASP:N	2.42	0.51
1:G:63:LYS:NZ	2:G:508:HOH:O	2.43	0.51
1:O:130:ILE:HG13	1:O:323:ARG:NH1	2.25	0.51
1:G:316:SER:HB2	1:G:338:THR:O	2.11	0.51
1:K:431:PHE:HB2	1:K:445:TRP:CZ2	2.45	0.51
1:M:287:THR:O	1:M:393:ASN:ND2	2.44	0.51
1:O:27:VAL:HG22	1:O:31:LEU:HD12	1.93	0.51
1:O:130:ILE:HG13	1:O:323:ARG:HH12	1.76	0.51
1:Q:378:ASN:HB3	1:Q:392:ILE:HD11	1.92	0.51
1:A:340:THR:OG1	1:A:343:ASP:HB2	2.11	0.51
1:B:10:ILE:HD11	1:B:367:GLN:OE1	2.11	0.51
1:B:307:VAL:HG13	1:G:327:ASN:HA	1.93	0.51
1:B:469:ASP:HB3	1:B:472:THR:HG22	1.93	0.51
1:I:228:CYS:HB2	1:I:247:MET:HG2	1.92	0.51
1:N:26:VAL:HA	1:N:29:THR:HG22	1.92	0.51
1:P:67:TRP:CE3	1:P:182:LYS:HE2	2.45	0.51
1:B:173:GLU:OE2	1:B:223:LYS:NZ	2.36	0.51
1:N:70:ILE:O	1:N:74:THR:HG23	2.11	0.51
1:P:171:LEU:HD11	1:P:175:TYR:CZ	2.45	0.51
1:C:272:ASN:O	1:C:276:MET:HG2	2.10	0.51
1:L:163:TYR:O	1:L:169:TYR:HE1	1.93	0.51
1:M:139:GLU:HG3	1:M:149:ARG:HG3	1.93	0.51
1:M:151:TRP:CE2	1:M:197:LYS:HD3	2.46	0.51
1:P:382:LEU:HA	1:P:385:GLN:NE2	2.26	0.51
1:E:460:PHE:CE1	1:K:130:ILE:HD11	2.46	0.51
1:H:124:ASP:HA	1:H:127:LYS:HD2	1.92	0.51
1:J:47:ASN:ND2	1:J:89:SER:OG	2.44	0.51
1:N:229:LEU:HD21	1:N:250:TYR:CZ	2.46	0.51
1:Q:286:ASP:OD1	1:Q:356:ARG:NH2	2.41	0.51
1:N:469:ASP:HB2	1:N:476:ARG:HD2	1.93	0.51
1:R:49:ASP:CB	1:R:158:GLN:HE22	2.24	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:127:LYS:NZ	1:C:123:ASP:OD2	2.43	0.50
1:L:144:ASP:OD1	1:L:146:THR:HG22	2.11	0.50
1:Q:381:GLU:O	1:Q:385:GLN:HG3	2.11	0.50
1:B:388:GLU:OE2	1:B:390:ARG:NH1	2.43	0.50
1:O:469:ASP:O	1:O:473:GLY:N	2.44	0.50
1:G:142:LEU:HB2	1:G:144:ASP:OD2	2.12	0.50
1:G:323:ARG:NE	2:G:511:HOH:O	2.44	0.50
1:N:12:TYR:CD1	1:N:15:ARG:HG2	2.45	0.50
1:O:285:LEU:HD13	1:O:341:PHE:CE2	2.47	0.50
1:A:469:ASP:CB	1:A:476:ARG:HE	2.25	0.50
1:E:414:LEU:O	1:E:418:MET:HG3	2.11	0.50
1:I:305:ILE:O	1:I:309:ILE:HG13	2.11	0.50
1:M:144:ASP:OD2	1:M:146:THR:OG1	2.24	0.50
1:O:289:ASP:HA	1:O:394:ARG:HH21	1.76	0.50
1:O:391:ASP:HA	1:O:394:ARG:HB2	1.92	0.50
1:I:230:PRO:HG2	1:I:247:MET:HE3	1.92	0.50
1:J:205:LEU:HD11	1:J:232:VAL:HG21	1.93	0.50
1:Q:131:ARG:O	1:Q:323:ARG:HB3	2.12	0.50
1:R:49:ASP:HB2	1:R:158:GLN:HE22	1.76	0.50
1:P:180:THR:HG21	1:P:224:HIS:HB3	1.94	0.50
1:B:133:GLU:O	1:R:460:PHE:HA	2.12	0.50
1:C:82:ASP:OD1	1:C:188:ARG:HD3	2.11	0.50
1:J:304:LYS:O	1:J:307:VAL:HG22	2.11	0.50
1:J:431:PHE:HE1	1:J:443:MET:HB3	1.77	0.50
1:P:144:ASP:CG	1:P:146:THR:H	2.15	0.50
1:H:215:ASP:OD1	1:H:245:ARG:HD3	2.12	0.50
1:L:166:ASP:OD1	1:L:170:GLN:NE2	2.44	0.50
1:L:179:LEU:O	1:L:184:VAL:HG13	2.12	0.50
1:M:382:LEU:HG	1:M:391:ASP:HB3	1.92	0.50
1:R:415:LEU:O	1:R:419:LYS:HD2	2.10	0.50
1:C:244:ARG:HA	1:C:279:ARG:HH22	1.76	0.49
1:R:61:ASP:O	1:R:64:VAL:HG22	2.11	0.49
1:D:242:ILE:HG23	1:D:247:MET:HB2	1.94	0.49
1:D:335:TYR:CD2	1:D:336:GLN:HG3	2.46	0.49
1:J:286:ASP:CG	1:J:369:TYR:HB3	2.32	0.49
1:J:303:GLU:CD	1:J:303:GLU:H	2.15	0.49
1:L:82:ASP:OD2	1:L:188:ARG:NH1	2.45	0.49
1:M:469:ASP:O	1:M:473:GLY:N	2.42	0.49
1:N:404:GLN:HG2	1:N:405:ASP:N	2.26	0.49
1:B:53:SER:O	1:B:89:SER:HB2	2.12	0.49
1:G:286:ASP:OD1	1:G:286:ASP:N	2.43	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:293:ILE:O	1:I:296:VAL:HG12	2.12	0.49
1:C:469:ASP:O	1:C:473:GLY:N	2.43	0.49
1:J:390:ARG:O	1:J:394:ARG:HG3	2.12	0.49
1:K:188:ARG:NH1	1:K:190:ASP:OD1	2.45	0.49
1:P:23:LEU:HD23	1:P:73:PHE:CZ	2.48	0.49
1:R:455:PHE:HB3	1:R:464:LYS:HG3	1.94	0.49
1:A:381:GLU:O	1:A:385:GLN:HG2	2.12	0.49
1:B:316:SER:HB2	1:B:338:THR:O	2.11	0.49
1:E:33:GLU:HB2	1:E:419:LYS:HE2	1.94	0.49
1:H:47:ASN:ND2	1:H:89:SER:OG	2.45	0.49
1:M:382:LEU:HD12	1:M:385:GLN:HE22	1.76	0.49
1:P:3:LEU:HD11	1:P:186:LEU:HD13	1.93	0.49
1:P:350:ASP:HB3	1:P:461:LYS:O	2.13	0.49
1:P:439:SER:HB3	2:P:509:HOH:O	2.11	0.49
1:P:467:TYR:CE2	1:P:476:ARG:HG3	2.47	0.49
1:Q:243:SER:HB2	1:Q:249:PRO:HG3	1.94	0.49
1:C:469:ASP:HB3	1:C:472:THR:CG2	2.42	0.49
1:E:58:LYS:HG2	1:E:178:PHE:CG	2.47	0.49
1:O:288:HIS:HA	1:O:369:TYR:CZ	2.47	0.49
1:P:15:ARG:HG2	1:P:370:TYR:OH	2.12	0.49
1:Q:374:LEU:HD22	1:Q:405:ASP:HB3	1.95	0.49
1:A:58:LYS:HG2	1:A:178:PHE:CD1	2.48	0.49
1:F:430:HIS:NE2	1:F:432:GLU:OE2	2.41	0.49
1:I:383:MET:HG2	1:I:388:GLU:O	2.13	0.49
1:Q:107:TYR:O	1:Q:110:LEU:HB3	2.13	0.49
1:F:258:LEU:HD13	1:F:355:ALA:HB1	1.95	0.49
1:G:253:ALA:O	1:G:256:PRO:HD2	2.13	0.49
1:K:17:GLY:HA3	1:K:22:ASP:HB3	1.93	0.49
1:L:430:HIS:CD2	1:L:446:ARG:HB3	2.48	0.49
1:P:88:ILE:HD11	1:P:111:PHE:CE1	2.48	0.49
1:B:279:ARG:HG3	1:B:280:ASN:N	2.26	0.49
1:K:176:ILE:HG22	1:K:224:HIS:CD2	2.48	0.49
1:N:9:LEU:HD23	1:N:38:LEU:HD11	1.93	0.49
1:P:97:ASP:OD2	1:P:105:SER:OG	2.23	0.49
1:Q:132:LYS:NZ	1:Q:154:PHE:O	2.44	0.49
1:R:171:LEU:HD11	1:R:175:TYR:CE2	2.48	0.49
1:R:400:GLU:H	1:R:400:GLU:CD	2.14	0.49
1:F:80:CYS:HA	1:F:186:LEU:O	2.13	0.49
1:H:112:VAL:HG22	1:H:162:ASN:HB2	1.94	0.49
1:O:8:GLN:HG2	1:0:37:GLY:HA3	1.94	0.49
1:0:132:LYS:HG3	1:0:134:LYS:0	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:472:THR:0	1:O:474:GLU:HG2	2.13	0.49
1:F:185:ASN:OD1	1:F:185:ASN:N	2.46	0.48
1:G:21:LYS:HE3	1:G:69:ASP:OD1	2.13	0.48
1:K:289:ASP:OD1	1:K:390:ARG:NH1	2.46	0.48
1:L:249:PRO:HD2	1:L:281:MET:HA	1.95	0.48
1:O:419:LYS:HB3	1:O:419:LYS:HE2	1.52	0.48
1:K:460:PHE:HA	1:L:133:GLU:O	2.13	0.48
1:L:432:GLU:HG3	1:L:444:ALA:HB3	1.94	0.48
1:P:139:GLU:OE2	1:P:147:LYS:HB3	2.12	0.48
1:P:382:LEU:HD13	1:P:395:HIS:HA	1.94	0.48
1:R:127:LYS:NZ	2:R:506:HOH:O	2.39	0.48
1:L:102:GLY:O	1:L:105:SER:HB3	2.14	0.48
1:Q:301:PRO:O	1:Q:305:ILE:HG13	2.12	0.48
1:R:85:VAL:O	1:R:161:LEU:HD23	2.13	0.48
1:E:249:PRO:HD2	1:E:281:MET:HA	1.95	0.48
1:J:33:GLU:HB2	1:J:419:LYS:HG2	1.95	0.48
1:Q:218:ASN:O	1:Q:222:LEU:HG	2.13	0.48
1:G:272:ASN:O	1:G:276:MET:HG2	2.14	0.48
1:L:33:GLU:HB3	1:L:419:LYS:HD2	1.95	0.48
1:L:244:ARG:HH11	1:L:244:ARG:HG3	1.78	0.48
1:M:142:LEU:HD12	1:M:146:THR:OG1	2.13	0.48
1:B:327:ASN:CB	1:R:307:VAL:HB	2.39	0.48
1:H:285:LEU:HD13	1:H:341:PHE:CE2	2.49	0.48
1:I:103:PHE:HZ	1:I:148:THR:HG21	1.78	0.48
1:A:397:TYR:OH	2:A:501:HOH:O	2.20	0.48
1:C:130:ILE:HG22	1:C:153:THR:HG23	1.94	0.48
1:E:388:GLU:OE2	1:E:390:ARG:HD3	2.13	0.48
1:F:308:LEU:O	1:F:312:ILE:HG12	2.14	0.48
1:O:110:LEU:HD11	1:O:161:LEU:HD22	1.96	0.48
1:R:287:THR:O	1:R:393:ASN:ND2	2.47	0.48
1:D:214:LEU:HG	1:D:247:MET:HE1	1.95	0.48
1:E:265:ALA:HB3	1:K:324:SER:HB2	1.95	0.48
1:K:135:GLU:HG2	1:K:136:PRO:HD2	1.94	0.48
1:N:9:LEU:HB3	1:N:38:LEU:HD12	1.95	0.48
1:0:24:TYR:HA	1:O:73:PHE:CZ	2.49	0.48
1:D:138:ARG:HD3	1:D:140:VAL:HG12	1.96	0.48
1:K:8:GLN:HG2	1:K:37:GLY:HA3	1.96	0.48
1:R:8:GLN:HA	1:R:37:GLY:O	2.13	0.48
1:R:474:GLU:O	1:R:474:GLU:HG3	2.13	0.48
1:C:469:ASP:CB	1:C:472:THR:HG22	2.44	0.48
1:C:472:THR:HG23	1:C:474:GLU:HB3	1.96	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:76:LYS:NZ	1:N:216:TRP:HE1	2.12	0.48
1:F:249:PRO:HD2	1:F:280:ASN:O	2.14	0.47
1:I:152:CYS:HB2	1:I:158:GLN:O	2.14	0.47
1:J:98:PHE:O	1:J:102:GLY:HA2	2.13	0.47
1:J:286:ASP:OD2	1:J:369:TYR:HB3	2.14	0.47
1:P:252:PHE:O	1:P:255:PRO:HD2	2.14	0.47
1:R:113:HIS:O	1:R:116:LYS:HG2	2.14	0.47
1:B:272:ASN:O	1:B:276:MET:HG2	2.14	0.47
1:F:254:LEU:HD13	1:F:273:TRP:CZ3	2.49	0.47
1:H:388:GLU:HG3	1:H:391:ASP:H	1.78	0.47
1:0:47:ASN:OD1	1:O:47:ASN:N	2.47	0.47
1:Q:15:ARG:NH1	1:Q:394:ARG:O	2.47	0.47
1:A:381:GLU:H	1:A:381:GLU:CD	2.17	0.47
1:B:450:TYR:CE1	1:B:470:VAL:HG12	2.50	0.47
1:F:42:PRO:O	2:F:501:HOH:O	2.20	0.47
1:F:324:SER:OG	2:F:502:HOH:O	2.20	0.47
1:G:82:ASP:OD1	1:G:188:ARG:HD3	2.14	0.47
1:I:154:PHE:O	1:I:158:GLN:HB2	2.15	0.47
1:P:182:LYS:HD2	1:P:182:LYS:N	2.28	0.47
1:A:81:VAL:HG22	1:A:184:VAL:HG11	1.96	0.47
1:H:38:LEU:HD22	1:H:40:ILE:CG1	2.44	0.47
1:H:252:PHE:O	1:H:255:PRO:HD2	2.14	0.47
1:I:12:TYR:CE2	1:I:394:ARG:HG2	2.49	0.47
1:I:241:ALA:O	1:I:245:ARG:HD2	2.14	0.47
1:P:138:ARG:O	1:P:138:ARG:HG3	2.14	0.47
1:P:356:ARG:HG3	1:P:414:LEU:HD13	1.96	0.47
1:A:469:ASP:HB2	1:A:476:ARG:HE	1.80	0.47
1:H:306:LYS:HE3	1:H:306:LYS:HB2	1.64	0.47
1:R:46:SER:CB	1:R:51:GLY:HA2	2.43	0.47
1:R:272:ASN:O	1:R:276:MET:HG2	2.15	0.47
1:H:110:LEU:HD11	1:H:161:LEU:HD22	1.97	0.47
1:I:12:TYR:HE2	1:I:394:ARG:HG2	1.80	0.47
1:K:151:TRP:CD2	1:K:197:LYS:HD3	2.50	0.47
1:L:286:ASP:OD2	1:L:286:ASP:N	2.45	0.47
1:M:57:HIS:CE1	1:M:84:THR:H	2.33	0.47
1:M:88:ILE:HG12	1:M:161:LEU:HD21	1.97	0.47
1:N:257:LEU:HD21	1:N:270:LEU:HA	1.97	0.47
1:N:404:GLN:HE21	1:N:404:GLN:HB3	1.49	0.47
1:P:123:ASP:O	1:P:127:LYS:HG3	2.14	0.47
1:Q:80:CYS:HA	1:Q:186:LEU:O	2.15	0.47
1:Q:88:ILE:HG12	1:Q:161:LEU:HD21	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:Q:242:ILE:O	1:Q:245:ARG:HB2	2.15	0.47
1:Q:349:ASP:CG	1:Q:410:VAL:HB	2.35	0.47
1:R:12:TYR:HB2	1:R:15:ARG:CG	2.43	0.47
1:R:92:SER:O	1:R:96:THR:HG23	2.14	0.47
1:R:240:TYR:O	1:R:244:ARG:HD3	2.14	0.47
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.67	0.47
1:H:382:LEU:HG	1:H:391:ASP:HB3	1.97	0.47
1:I:239:GLN:NE2	1:I:250:TYR:H	2.13	0.47
1:R:235:HIS:HD2	1:R:297:GLU:OE1	1.98	0.47
1:A:53:SER:O	1:A:89:SER:HB2	2.15	0.47
1:G:47:ASN:ND2	1:G:89:SER:OG	2.34	0.47
1:G:466:THR:HG23	1:G:475:THR:HG23	1.96	0.47
1:J:457:ASP:HB3	1:J:462:THR:CG2	2.45	0.47
1:P:41:LEU:HD21	1:P:288:HIS:CG	2.50	0.47
1:E:138:ARG:HH11	1:E:159:ILE:HD11	1.80	0.47
1:E:466:THR:HG22	1:E:477:HIS:CD2	2.50	0.47
1:G:244:ARG:HG3	1:G:244:ARG:HH11	1.80	0.47
1:J:472:THR:HG21	1:J:476:ARG:HH22	1.80	0.47
1:K:330:SER:O	1:K:334:ILE:HD12	2.14	0.47
1:L:58:LYS:HG2	1:L:178:PHE:CG	2.50	0.47
1:L:62:PRO:HG2	1:R:63:LYS:HG2	1.97	0.47
1:L:79:LEU:HD23	1:L:184:VAL:HG12	1.97	0.47
1:A:400:GLU:HG3	1:A:404:GLN:NE2	2.28	0.46
1:E:91:GLU:OE2	2:E:502:HOH:O	2.21	0.46
1:G:404:GLN:NE2	1:L:404:GLN:O	2.42	0.46
1:H:132:LYS:HD3	1:H:153:THR:O	2.15	0.46
1:H:192:PHE:CE1	1:H:214:LEU:HD11	2.50	0.46
1:J:472:THR:HG21	1:J:476:ARG:NH2	2.30	0.46
1:P:59:GLU:HA	1:P:67:TRP:HE1	1.80	0.46
1:R:12:TYR:CD2	1:R:15:ARG:HG2	2.50	0.46
1:R:207:GLU:HG2	1:R:211:TYR:CE2	2.49	0.46
1:B:80:CYS:HA	1:B:186:LEU:O	2.15	0.46
1:L:236:THR:N	2:L:507:HOH:O	2.44	0.46
1:O:87:HIS:CD2	1:O:158:GLN:HG2	2.50	0.46
1:0:240:TYR:O	1:O:244:ARG:HG2	2.15	0.46
1:O:286:ASP:HB3	1:O:341:PHE:HB2	1.97	0.46
1:C:79:LEU:HD23	1:C:184:VAL:HG22	1.96	0.46
1:D:14:ASP:OD1	1:D:14:ASP:N	2.47	0.46
1:D:385:GLN:H	1:D:385:GLN:HG3	1.57	0.46
1:H:303:GLU:HG3	1:H:304:LYS:N	2.30	0.46
1:J:306:LYS:HG3	1:J:331:VAL:HG23	1.98	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:218:ASN:HB2	1:L:247:MET:CE	2.45	0.46
1:M:215:ASP:O	1:M:219:GLN:HG2	2.15	0.46
1:N:222:LEU:HD12	1:N:226:ALA:O	2.16	0.46
1:A:474:GLU:CG	1:A:476:ARG:HD3	2.44	0.46
1:D:249:PRO:HD2	1:D:281:MET:HA	1.98	0.46
1:G:236:THR:HG22	2:G:574:HOH:O	2.14	0.46
1:K:88:ILE:HG12	1:K:161:LEU:HD21	1.97	0.46
1:R:464:LYS:HB2	1:R:464:LYS:HE3	1.54	0.46
1:E:479:GLU:O	1:E:480:CYS:C	2.54	0.46
1:F:33:GLU:HB2	1:F:419:LYS:HD3	1.98	0.46
1:P:2:LEU:HD23	1:P:227:GLU:HB2	1.98	0.46
1:R:29:THR:HB	1:R:30:HIS:ND1	2.30	0.46
1:A:237:SER:HB3	1:B:276:MET:SD	2.55	0.46
1:B:205:LEU:HD21	1:B:232:VAL:HG11	1.96	0.46
1:E:241:ALA:O	1:E:245:ARG:HG3	2.16	0.46
1:J:31:LEU:HD13	1:J:35:ILE:HD13	1.97	0.46
1:K:9:LEU:HD23	1:K:38:LEU:HD11	1.97	0.46
1:M:466:THR:HG22	1:M:477:HIS:ND1	2.30	0.46
1:N:241:ALA:O	1:N:245:ARG:HD2	2.15	0.46
1:O:3:LEU:HD11	1:O:186:LEU:HD13	1.96	0.46
1:Q:12:TYR:CB	1:Q:15:ARG:HG2	2.45	0.46
1:E:69:ASP:OD1	2:E:503:HOH:O	2.21	0.46
1:G:472:THR:HG22	1:G:474:GLU:HB3	1.97	0.46
1:J:2:LEU:HG	1:J:227:GLU:OE2	2.15	0.46
1:N:58:LYS:HE3	1:N:174:SER:OG	2.16	0.46
1:O:402:VAL:O	1:O:406:ILE:HG12	2.16	0.46
1:Q:179:LEU:O	1:Q:184:VAL:HG13	2.15	0.46
1:E:80:CYS:HB2	1:E:186:LEU:HB3	1.97	0.46
1:N:389:LEU:O	1:N:392:ILE:HG23	2.15	0.46
1:Q:269:TYR:N	2:Q:509:HOH:O	2.48	0.46
1:R:13:PRO:HG2	1:R:43:PHE:HB3	1.97	0.46
1:D:327:ASN:O	1:D:330:SER:HB3	2.16	0.46
1:E:10:ILE:HD11	1:E:367:GLN:HB3	1.98	0.46
1:L:10:ILE:HD11	1:L:367:GLN:HB3	1.97	0.46
1:P:381:GLU:H	1:P:381:GLU:CD	2.19	0.46
1:Q:231:GLU:O	1:Q:231:GLU:HG3	2.15	0.46
1:Q:278:PRO:HD2	1:Q:281:MET:HE3	1.98	0.46
1:R:7:VAL:HG12	1:R:35:ILE:HG22	1.98	0.46
1:H:130:ILE:HG22	1:H:153:THR:HG23	1.98	0.46
1:I:239:GLN:HG3	1:I:249:PRO:CB	2.42	0.46
1:0:213:ILE:0	1:O:217:VAL:HG23	2.16	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:O:453:HIS:HD2	2:O:530:HOH:O	1.98	0.46
1:R:39:HIS:HB2	1:R:80:CYS:HB3	1.98	0.46
1:B:12:TYR:HB2	1:B:15:ARG:HG2	1.98	0.45
1:C:270:LEU:HD23	1:C:441:VAL:HG21	1.97	0.45
1:D:123:ASP:O	1:D:127:LYS:HG3	2.16	0.45
1:F:142:LEU:HD12	1:F:146:THR:HB	1.98	0.45
1:F:328:ILE:HG12	1:O:311:ASN:HA	1.97	0.45
1:H:196:THR:OG1	2:H:501:HOH:O	2.21	0.45
1:H:382:LEU:O	1:H:385:GLN:HG3	2.16	0.45
1:I:406:ILE:HA	1:I:411:VAL:HG11	1.97	0.45
1:L:399:LEU:O	1:L:403:GLU:HG2	2.15	0.45
1:L:439:SER:OG	1:L:459:ASN:OD1	2.32	0.45
1:M:45:PRO:HA	2:M:507:HOH:O	2.16	0.45
1:M:192:PHE:CE1	1:M:214:LEU:HD11	2.51	0.45
1:N:130:ILE:HD13	1:N:136:PRO:HG3	1.98	0.45
1:O:82:ASP:HB3	1:O:190:ASP:OD2	2.16	0.45
1:O:215:ASP:O	1:O:219:GLN:HG3	2.16	0.45
1:P:255:PRO:HB2	1:P:256:PRO:HD3	1.97	0.45
1:Q:160:ASP:OD2	1:Q:197:LYS:NZ	2.47	0.45
1:G:285:LEU:HD13	1:G:341:PHE:CE2	2.51	0.45
1:H:286:ASP:HB3	1:H:341:PHE:HB2	1.98	0.45
1:I:140:VAL:HG22	1:I:148:THR:O	2.16	0.45
1:L:16:ILE:HG23	1:L:402:VAL:HG21	1.96	0.45
1:N:139:GLU:CD	1:N:147:LYS:HE3	2.36	0.45
1:A:454:LEU:HD11	1:A:456:VAL:HG23	1.98	0.45
1:H:47:ASN:ND2	1:H:91:GLU:HG3	2.26	0.45
1:J:243:SER:OG	1:J:279:ARG:HG3	2.15	0.45
1:K:202:SER:O	1:K:203:CYS:HB2	2.15	0.45
1:N:9:LEU:HB3	1:N:38:LEU:CD1	2.46	0.45
1:P:441:VAL:HG13	1:P:456:VAL:HB	1.98	0.45
1:Q:325:ALA:HB1	1:Q:333:ALA:HB1	1.98	0.45
1:Q:331:VAL:HG23	1:Q:332:GLY:N	2.32	0.45
1:A:38:LEU:CD2	1:A:40:ILE:CG1	2.94	0.45
1:A:88:ILE:HG12	1:A:161:LEU:HD21	1.99	0.45
1:F:130:ILE:HD11	1:O:460:PHE:HE1	1.82	0.45
1:H:272:ASN:O	1:H:276:MET:HG2	2.17	0.45
1:J:382:LEU:O	1:J:385:GLN:HG2	2.17	0.45
1:K:391:ASP:HA	1:K:394:ARG:HB2	1.97	0.45
1:L:12:TYR:CB	1:L:15:ARG:HG2	2.46	0.45
1:L:38:LEU:HD23	1:L:38:LEU:HA	1.78	0.45
1:L:382:LEU:HG	1:L:391:ASP:HB3	1.98	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:R:406:ILE:HD12	1:R:415:LEU:HD11	1.99	0.45
1:M:252:PHE:O	1:M:255:PRO:HD2	2.17	0.45
1:N:79:LEU:HD23	1:N:184:VAL:HG22	1.98	0.45
1:P:285:LEU:HD13	1:P:341:PHE:CE2	2.51	0.45
1:Q:112:VAL:HG22	1:Q:162:ASN:HB2	1.98	0.45
1:R:12:TYR:HB2	1:R:15:ARG:CB	2.44	0.45
1:R:19:ASN:OD1	1:R:21:LYS:HB2	2.16	0.45
1:C:293:ILE:O	1:C:296:VAL:HG12	2.17	0.45
1:J:177:GLY:HA2	1:J:224:HIS:CD2	2.52	0.45
1:K:169:TYR:HB3	1:K:216:TRP:CZ2	2.51	0.45
1:D:257:LEU:HD21	1:D:270:LEU:HA	1.99	0.45
1:H:467:TYR:CE2	1:H:476:ARG:HD3	2.51	0.45
1:I:81:VAL:HG22	1:I:184:VAL:HG11	1.99	0.45
1:K:453:HIS:HB3	1:K:466:THR:OG1	2.16	0.45
1:L:12:TYR:O	2:L:501:HOH:O	2.21	0.45
1:P:285:LEU:HB2	1:P:356:ARG:NH1	2.32	0.45
1:D:385:GLN:HE21	1:D:385:GLN:HB2	1.47	0.45
1:F:252:PHE:O	1:F:255:PRO:HD2	2.17	0.45
1:G:100:ALA:HA	1:G:143:SER:OG	2.17	0.45
1:J:95:PHE:CE2	1:J:99:ILE:HD11	2.51	0.45
1:K:128:ILE:HA	1:K:202:SER:O	2.17	0.45
1:N:15:ARG:HG3	1:N:370:TYR:OH	2.16	0.45
1:O:218:ASN:ND2	1:O:247:MET:HG3	2.31	0.45
1:O:345:LEU:HD23	1:O:345:LEU:HA	1.86	0.45
1:Q:53:SER:O	1:Q:89:SER:HB2	2.17	0.45
1:Q:130:ILE:CD1	1:Q:136:PRO:HG3	2.44	0.45
1:Q:322:ARG:NH1	1:Q:334:ILE:O	2.50	0.45
1:D:120:ILE:HG22	1:D:125:MET:HG2	1.99	0.45
1:G:192:PHE:HE1	1:G:232:VAL:HG22	1.81	0.45
1:L:308:LEU:HD12	1:L:312:ILE:HD13	1.99	0.45
1:L:383:MET:HE3	1:L:383:MET:HB3	1.86	0.45
1:M:388:GLU:HG3	1:M:391:ASP:H	1.82	0.45
1:M:469:ASP:HB3	1:M:472:THR:HB	1.97	0.45
1:B:323:ARG:NH2	2:B:505:HOH:O	2.42	0.45
1:C:460:PHE:CE1	1:D:130:ILE:HD11	2.51	0.45
1:H:12:TYR:CD1	1:H:15:ARG:HG2	2.52	0.45
1:K:209:GLU:CD	1:K:209:GLU:H	2.20	0.45
1:L:380:HIS:CD2	1:L:392:ILE:HD11	2.52	0.45
1:N:110:LEU:HD23	1:N:111:PHE:CZ	2.52	0.45
1:N:135:GLU:HB3	1:N:137:PHE:CE1	2.52	0.45
1:O:389:LEU:O	1:O:392:ILE:HG22	2.17	0.45



	A h O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:237:SER:HB2	1:G:275:ARG:HB3	1.98	0.44
1:I:252:PHE:O	1:I:255:PRO:HD2	2.16	0.44
1:K:38:LEU:HD13	1:K:38:LEU:HA	1.83	0.44
1:L:70:ILE:O	1:L:74:THR:HG23	2.17	0.44
1:M:16:ILE:HG23	1:M:402:VAL:HG21	1.99	0.44
1:M:94:GLU:OE1	1:M:94:GLU:N	2.43	0.44
1:O:151:TRP:N	2:O:511:HOH:O	2.50	0.44
1:A:177:GLY:HA2	1:A:224:HIS:CD2	2.51	0.44
1:B:123:ASP:OD1	2:B:501:HOH:O	2.21	0.44
1:N:57:HIS:HB2	1:N:175:TYR:CD1	2.52	0.44
1:P:41:LEU:HB3	1:P:42:PRO:HD2	1.99	0.44
1:P:322:ARG:HH12	1:P:334:ILE:C	2.20	0.44
1:A:244:ARG:NH1	1:A:244:ARG:HG3	2.33	0.44
1:B:12:TYR:CD2	1:B:15:ARG:HG2	2.52	0.44
1:C:476:ARG:CZ	1:C:476:ARG:HB3	2.48	0.44
1:J:192:PHE:CE1	1:J:214:LEU:HD11	2.52	0.44
1:K:33:GLU:CB	1:K:419:LYS:HG2	2.43	0.44
1:O:452:CYS:HA	1:O:466:THR:O	2.18	0.44
1:P:469:ASP:O	1:P:473:GLY:N	2.40	0.44
1:Q:385:GLN:HG3	1:Q:385:GLN:H	1.58	0.44
1:R:101:ASN:HB2	1:R:105:SER:HB2	1.99	0.44
1:A:185:ASN:OD1	1:A:185:ASN:N	2.48	0.44
1:E:265:ALA:HB2	1:K:324:SER:HB2	1.99	0.44
1:M:286:ASP:HB3	1:M:341:PHE:HB2	1.99	0.44
1:Q:449:ASP:HB3	1:Q:470:VAL:HG12	1.98	0.44
1:J:15:ARG:HG2	1:J:370:TYR:OH	2.18	0.44
1:M:20:LEU:HD12	1:M:64:VAL:HG23	1.99	0.44
1:M:76:LYS:HE2	1:M:76:LYS:HB3	1.73	0.44
1:O:244:ARG:HA	1:O:244:ARG:HD3	1.91	0.44
1:P:19:ASN:O	1:P:22:ASP:HB2	2.18	0.44
1:P:425:PRO:HG2	1:P:450:TYR:CE1	2.53	0.44
1:R:68:ASP:HA	1:R:71:GLU:HG3	1.99	0.44
1:A:244:ARG:HG3	1:A:244:ARG:HH11	1.81	0.44
1:H:152:CYS:HB2	1:H:158:GLN:O	2.18	0.44
1:H:205:LEU:HD11	1:H:232:VAL:HG21	1.99	0.44
1:I:10:ILE:HD12	1:I:39:HIS:HD2	1.82	0.44
1:L:12:TYR:CG	1:L:15:ARG:HG2	2.53	0.44
1:L:15:ARG:HG3	1:L:370:TYR:OH	2.17	0.44
1:P:406:ILE:HA	1:P:411:VAL:HG11	1.98	0.44
1:E:53:SER:O	1:E:89:SER:HB2	2.17	0.44
1:F:1:MET:HG2	1:F:3:LEU:O	2.18	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:P:144:ASP:OD2	1:P:146:THR:HB	2.18	0.44
1:R:156:GLU:H	1:R:156:GLU:HG2	1.58	0.44
1:R:381:GLU:H	1:R:381:GLU:HG2	1.43	0.44
1:R:391:ASP:HA	1:R:394:ARG:HG3	1.98	0.44
1:F:382:LEU:HG	1:F:391:ASP:HB3	2.00	0.44
1:G:81:VAL:HG21	1:G:179:LEU:HD22	1.99	0.44
1:G:315:ARG:HD2	1:G:343:ASP:O	2.18	0.44
1:L:219:GLN:HG3	1:L:220:VAL:N	2.32	0.44
1:N:29:THR:HG23	1:N:30:HIS:CG	2.52	0.44
1:R:450:TYR:CE2	1:R:470:VAL:HG22	2.53	0.44
1:D:67:TRP:CE3	1:D:182:LYS:HG3	2.53	0.44
1:D:272:ASN:O	1:D:276:MET:HG2	2.18	0.44
1:I:252:PHE:O	2:I:501:HOH:O	2.21	0.44
1:O:407:GLN:O	1:O:408:LYS:C	2.56	0.44
1:P:381:GLU:HA	1:P:384:GLU:HG2	2.00	0.44
1:Q:191:ALA:HB1	1:Q:194:TYR:HD2	1.83	0.44
1:R:8:GLN:HG2	1:R:37:GLY:HA3	2.00	0.44
1:D:207:GLU:HG2	1:D:211:TYR:CE2	2.53	0.43
1:E:88:ILE:HG12	1:E:161:LEU:HD21	1.99	0.43
1:E:285:LEU:HD13	1:E:341:PHE:CE2	2.53	0.43
1:F:53:SER:O	1:F:89:SER:HB2	2.17	0.43
1:K:61:ASP:O	1:K:64:VAL:HG22	2.17	0.43
1:O:109:ASP:HB2	1:O:167:LEU:HD12	1.99	0.43
1:P:34:ALA:HB1	1:P:418:MET:HE2	1.98	0.43
1:R:53:SER:HB2	1:R:158:GLN:NE2	2.33	0.43
1:C:177:GLY:HA2	1:C:224:HIS:CD2	2.53	0.43
1:J:179:LEU:O	1:J:184:VAL:HG13	2.18	0.43
1:0:82:ASP:OD2	1:O:188:ARG:HD3	2.18	0.43
1:0:116:LYS:HE2	1:O:117:PHE:CE2	2.52	0.43
1:O:322:ARG:HG2	1:O:335:TYR:HB2	2.00	0.43
1:P:147:LYS:HB2	1:P:147:LYS:HE3	1.39	0.43
1:Q:74:THR:HG21	1:Q:182:LYS:O	2.19	0.43
1:B:254:LEU:HD11	1:B:258:LEU:HD22	1.99	0.43
1:C:399:LEU:HA	1:C:399:LEU:HD23	1.75	0.43
1:E:133:GLU:H	1:E:134:LYS:HZ2	1.66	0.43
1:E:459:ASN:HB3	1:K:323:ARG:NH1	2.33	0.43
1:H:188:ARG:NH1	1:H:190:ASP:OD1	2.47	0.43
1:L:293:ILE:O	1:L:296:VAL:HG12	2.19	0.43
1:L:303:GLU:HA	1:L:303:GLU:OE1	2.18	0.43
1:O:29:THR:HG23	1:O:30:HIS:CG	2.53	0.43
1:P:141:THR:CG2	1:P:145:GLY:HA2	2.48	0.43


		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:P:292:CYS:SG	1:P:294:PRO:HD2	2.58	0.43	
1:P:303:GLU:HG2	2:P:535:HOH:O	2.18	0.43	
1:Q:380:HIS:O	1:Q:384:GLU:HG2	2.17	0.43	
1:R:315:ARG:HD3	1:R:346:MET:HG2	2.00	0.43	
1:B:207:GLU:HG2	1:B:211:TYR:CE2	2.54	0.43	
1:C:409:PRO:O	1:C:413:ARG:HG3	2.17	0.43	
1:K:79:LEU:CD2	1:K:184:VAL:HG12	2.48	0.43	
1:K:127:LYS:HE2	1:K:127:LYS:HB2	1.51	0.43	
1:P:308:LEU:O	1:P:312:ILE:HG12	2.17	0.43	
1:Q:241:ALA:O	1:Q:245:ARG:HG2	2.18	0.43	
1:R:79:LEU:HD13	1:R:81:VAL:HG13	1.99	0.43	
1:G:287:THR:O	1:G:393:ASN:ND2	2.51	0.43	
1:L:130:ILE:HG22	1:L:153:THR:HG23	2.00	0.43	
1:L:277:CYS:O	1:L:279:ARG:NH2	2.52	0.43	
1:M:70:ILE:O	1:M:74:THR:HG23	2.18	0.43	
1:R:153:THR:HG23	1:R:154:PHE:CD1	2.54	0.43	
1:A:309:ILE:HD13	1:A:334:ILE:HG13	2.01	0.43	
1:B:81:VAL:HG22	1:B:184:VAL:HG11	2.00	0.43	
1:F:88:ILE:HG12	1:F:161:LEU:HD21	2.00	0.43	
1:G:323:ARG:NH2	2:G:511:HOH:O	2.51	0.43	
1:M:57:HIS:HE1	1:M:84:THR:H	1.66	0.43	
1:O:97:ASP:HB3	1:0:107:TYR:HD2	1.84	0.43	
1:P:240:TYR:CE1	1:P:278:PRO:HG3	2.53	0.43	
1:R:450:TYR:HE2	1:R:470:VAL:HG13	1.84	0.43	
1:A:16:ILE:HG23	1:A:402:VAL:HG21	2.00	0.43	
1:D:63:LYS:HB3	1:D:63:LYS:HE3	1.84	0.43	
1:E:132:LYS:HG2	2:E:508:HOH:O	2.18	0.43	
1:H:74:THR:HG21	1:H:182:LYS:O	2.18	0.43	
1:K:258:LEU:HD21	1:K:358:ILE:HG21	2.00	0.43	
1:K:449:ASP:OD1	1:K:449:ASP:N	2.50	0.43	
1:R:321:MET:HE3	1:R:321:MET:HB3	1.95	0.43	
1:B:109:ASP:OD2	1:B:165:SER:HB2	2.19	0.43	
1:B:213:ILE:O	1:B:217:VAL:HG23	2.18	0.43	
1:E:322:ARG:HD3	1:E:335:TYR:HB2	2.01	0.43	
1:K:43:PHE:HE2	1:K:67:TRP:CH2	2.36	0.43	
1:K:179:LEU:O	1:K:184:VAL:HG13	2.19	0.43	
1:K:292:CYS:SG	1:K:294:PRO:HD2	2.58	0.43	
1:M:417:LEU:HD23	1:M:417:LEU:HA	1.85	0.43	
1:Q:254:LEU:HD13	1:Q:273:TRP:CZ3	2.54	0.43	
1:Q:293:ILE:HD11	1:Q:337:LEU:HD11	2.00	0.43	
1:A:413:ARG:NE	1:A:480:CYS:OXT	2.32	0.43	



			Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:240:TYR:O	1:D:244:ARG:HD3	2.18	0.43	
1:F:312:ILE:HD13	1:F:315:ARG:NH2	2.34	0.43	
1:L:257:LEU:HD21	1:L:270:LEU:HA	2.00	0.43	
1:O:76:LYS:HD3	1:0:77:TYR:CZ	2.53	0.43	
1:P:116:LYS:HE3	1:P:117:PHE:CZ	2.53	0.43	
1:P:249:PRO:HD3	1:P:280:ASN:HD22	1.83	0.43	
1:R:2:LEU:HD12	1:R:3:LEU:HG	2.01	0.43	
1:R:44:PHE:HB2	1:R:54:PRO:HB3	2.01	0.43	
1:R:478:LEU:HD12	1:R:479:GLU:N	2.33	0.43	
1:A:95:PHE:CE2	1:A:99:ILE:HD11	2.53	0.43	
1:A:469:ASP:O	1:A:473:GLY:N	2.44	0.43	
1:C:152:CYS:HA	1:C:160:ASP:OD1	2.19	0.43	
1:D:125:MET:HA	1:D:128:ILE:HD12	2.01	0.43	
1:D:327:ASN:ND2	1:D:330:SER:HB2	2.34	0.43	
1:F:135:GLU:HG2	1:O:460:PHE:CD1	2.53	0.43	
1:I:306:LYS:HE2	1:I:310:ASP:OD1	2.19	0.43	
1:I:424:TYR:HA	1:I:425:PRO:HD3	1.91	0.43	
1:M:209:GLU:OE1	1:M:209:GLU:N	2.51	0.43	
1:N:439:SER:O	1:N:458:LEU:HB2	2.17	0.43	
1:O:218:ASN:O	1:O:222:LEU:HG	2.19	0.43	
1:C:395:HIS:NE2	1:C:396:TYR:O	2.52	0.42	
1:I:70:ILE:HD13	1:I:70:ILE:HA	1.87	0.42	
1:L:61:ASP:OD1	1:L:64:VAL:HG13	2.19	0.42	
1:O:23:LEU:HG	1:O:73:PHE:HZ	1.83	0.42	
1:R:66:THR:HG23	1:R:68:ASP:H	1.83	0.42	
1:B:382:LEU:HG	1:B:391:ASP:HB3	2.00	0.42	
1:G:425:PRO:HG2	1:G:450:TYR:CE2	2.54	0.42	
1:I:381:GLU:O	1:I:385:GLN:HG3	2.19	0.42	
1:N:154:PHE:HB2	1:N:155:THR:H	1.63	0.42	
1:N:408:LYS:HB2	1:N:408:LYS:HE3	1.74	0.42	
1:O:172:MET:HA	1:O:172:MET:CE	2.47	0.42	
1:R:4:LYS:HD2	1:R:78:ASP:CG	2.40	0.42	
1:R:66:THR:HG22	1:R:69:ASP:CG	2.39	0.42	
1:B:316:SER:HB3	1:B:339:CYS:HB3	2.01	0.42	
1:B:429:GLY:HA3	1:B:446:ARG:O	2.19	0.42	
1:D:12:TYR:N	2:D:510:HOH:O	2.44	0.42	
1:D:252:PHE:O	1:D:255:PRO:HD2	2.19	0.42	
1:D:284:VAL:O	1:D:285:LEU:HD23	2.20	0.42	
1:G:446:ARG:HB2	1:G:451:TYR:HD1	1.84	0.42	
1:L:31:LEU:HB3	1:L:35:ILE:HG12	2.02	0.42	
1:L:267:SER:O	1:L:271:LYS:HG3	2.20	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:R:265:ALA:HA	265:ALA:HA 1:R:458:LEU:HB3		0.42	
1:R:456:VAL:HG22	1:R:463:VAL:HG22	2.01	0.42	
1:C:350:ASP:HB3	1:C:461:LYS:O	2.19	0.42	
1:C:459:ASN:ND2	2:C:528:HOH:O	2.51	0.42	
1:G:360:PHE:HD1	1:G:417:LEU:HD22	1.84	0.42	
1:J:71:GLU:HA	1:J:74:THR:OG1	2.20	0.42	
1:K:110:LEU:HD23	1:K:111:PHE:CZ	2.55	0.42	
1:N:286:ASP:HB3	1:N:341:PHE:HB2	2.02	0.42	
1:O:20:LEU:HD12	1:O:65:GLY:HA3	2.00	0.42	
1:P:382:LEU:O	1:P:386:SER:HB3	2.19	0.42	
1:R:421:ARG:HA	1:R:427:PHE:CE2	2.54	0.42	
1:B:12:TYR:HB2	1:B:15:ARG:HB2	2.01	0.42	
1:B:292:CYS:SG	1:B:294:PRO:HD2	2.58	0.42	
1:B:474:GLU:H	1:B:474:GLU:HG2	1.69	0.42	
1:D:130:ILE:HG22	1:D:153:THR:HG23	2.00	0.42	
1:D:379:ASP:OD2	1:D:395:HIS:HD2	2.02	0.42	
1:E:432:GLU:HG3	1:E:444:ALA:HB3	2.01	0.42	
1:F:100:ALA:HA	1:F:143:SER:HB3	2.01	0.42	
1:G:15:ARG:HD3	1:G:396:TYR:CE2	2.54	0.42	
1:G:378:ASN:HB3	1:G:392:ILE:HG12	2.01	0.42	
1:L:458:LEU:O	1:L:461:LYS:NZ	2.34	0.42	
1:O:70:ILE:H	:70:ILE:H 1:O:70:ILE:HG12		0.42	
1:P:142:LEU:HD12	1:P:146:THR:HG22	2.02	0.42	
1:P:381:GLU:O	1:P:384:GLU:HB2	2.20	0.42	
1:Q:309:ILE:HG21	1:Q:334:ILE:HD12	2.01	0.42	
1:R:47:ASN:ND2	1:R:90:ASP:OD1	2.52	0.42	
1:R:207:GLU:HG2	1:R:211:TYR:HE2	1.83	0.42	
1:E:424:TYR:HA	1:E:425:PRO:HD3	1.92	0.42	
1:I:309:ILE:HG23	1:I:337:LEU:HD21	2.01	0.42	
1:L:76:LYS:HE2	1:L:76:LYS:HB3	1.72	0.42	
1:L:325:ALA:CB	1:L:333:ALA:HA	2.48	0.42	
1:M:60:VAL:HG23	1:M:67:TRP:CD2	2.55	0.42	
1:N:285:LEU:HD13	1:N:341:PHE:CE2	2.55	0.42	
1:O:247:MET:HE2	1:O:247:MET:HB2	1.66	0.42	
1:R:31:LEU:O	1:R:35:ILE:HG13	2.19	0.42	
1:R:326:ALA:O	1:R:328:ILE:HG23	2.18	0.42	
1:A:424:TYR:HA	1:A:425:PRO:HD3	1.86	0.42	
1:B:469:ASP:OD2	1:B:471:GLU:HG2	2.20	0.42	
1:F:319:PRO:HG2	1:F:321:MET:HE1	2.01	0.42	
1:H:219:GLN:NE2	2:H:515:HOH:O	2.53	0.42	
1:K:67:TRP:CE3	1:K:182:LYS:HG3	2.55	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:241:ALA:O	1:K:241:ALA:O 1:K:245:ARG:HD2		0.42
1:L:178:PHE:CE1	1:L:182:LYS:HE3	2.55	0.42
1:M:219:GLN:O	1:M:223:LYS:HG2	2.19	0.42
1:M:380:HIS:HA	1:M:383:MET:HE2	2.01	0.42
1:O:133:GLU:HA	1:O:323:ARG:HD2	2.01	0.42
1:O:278:PRO:HG2	1:O:281:MET:SD	2.60	0.42
1:Q:37:GLY:O	1:Q:38:LEU:HD12	2.20	0.42
1:R:312:ILE:O	1:R:316:SER:HB3	2.19	0.42
1:B:15:ARG:HD2	1:B:396:TYR:CD2	2.54	0.42
1:H:407:GLN:HA	1:H:412:GLN:HE21	1.84	0.42
1:K:219:GLN:H	1:K:219:GLN:HG3	1.72	0.42
1:K:400:GLU:H	1:K:400:GLU:CD	2.23	0.42
1:L:279:ARG:H	1:L:279:ARG:HG2	1.50	0.42
1:C:16:ILE:N	2:C:513:HOH:O	2.37	0.42
1:G:441:VAL:HG13	1:G:456:VAL:HB	2.02	0.42
1:H:263:LEU:HD23	1:H:263:LEU:HA	1.86	0.42
1:H:399:LEU:O	1:H:403:GLU:HG2	2.19	0.42
1:I:223:LYS:HB3	1:I:223:LYS:HE2	1.51	0.42
1:K:430:HIS:CE1	1:K:446:ARG:HB3	2.54	0.42
1:M:15:ARG:HG2	1:M:370:TYR:OH	2.20	0.42
1:N:15:ARG:HA	1:N:15:ARG:HD3	1.77	0.42
1:P:88:ILE:HD11	1:P:111:PHE:HE1	1.83	0.42
1:Q:110:LEU:HD11	1:Q:161:LEU:HD22	2.02	0.42
1:B:18:ASN:O	1:K:63:LYS:HE3	2.19	0.42
1:B:450:TYR:HE1	1:B:470:VAL:HG12	1.85	0.42
1:E:80:CYS:HA	1:E:186:LEU:O	2.20	0.42
1:E:286:ASP:OD1	1:E:286:ASP:N	2.53	0.42
1:F:79:LEU:HD23	1:F:184:VAL:HG12	2.02	0.42
1:G:38:LEU:HD23	1:G:38:LEU:HA	1.85	0.42
1:H:395:HIS:NE2	1:H:396:TYR:O	2.52	0.42
1:I:134:LYS:H	1:I:134:LYS:HG2	1.53	0.42
1:J:454:LEU:HD11	1:J:456:VAL:HG23	2.01	0.42
1:L:390:ARG:HD2	1:L:394:ARG:NH2	2.35	0.42
1:M:230:PRO:HG3	1:M:247:MET:HE2	2.02	0.42
1:N:82:ASP:OD2	1:N:188:ARG:HD3	2.19	0.42
1:N:132:LYS:HE3	1:N:134:LYS:HD3	2.00	0.42
1:Q:87:HIS:CD2	1:Q:158:GLN:HG2	2.55	0.42
1:R:79:LEU:HD23	1:R:79:LEU:HA	1.86	0.42
1:C:233:HIS:HA	1:C:295:ASP:OD2	2.20	0.41
1:E:39:HIS:HD2	2:E:501:HOH:O	2.02	0.41
1:E:324:SER:O	1:E:325:ALA:HB3	2.20	0.41



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:P:63:LYS:HE2	1:P:63:LYS:HE2 1:P:63:LYS:HB3		0.41	
1:P:421:ARG:HA	1:P:427:PHE:CE2	2.55	0.41	
1:A:267:SER:O	1:A:271:LYS:HG3	2.20	0.41	
1:B:277:CYS:HB2	1:B:281:MET:HE1	2.01	0.41	
1:C:207:GLU:HG2	1:C:211:TYR:CE2	2.55	0.41	
1:C:236:THR:HG22	2:C:591:HOH:O	2.20	0.41	
1:C:240:TYR:CZ	1:C:278:PRO:HG3	2.54	0.41	
1:C:431:PHE:HB2	1:C:445:TRP:CH2	2.55	0.41	
1:F:218:ASN:O	1:F:222:LEU:HD13	2.20	0.41	
1:I:103:PHE:CZ	1:I:148:THR:HG21	2.54	0.41	
1:J:409:PRO:O	1:J:413:ARG:HG3	2.21	0.41	
1:K:301:PRO:O	1:K:305:ILE:HG13	2.19	0.41	
1:P:162:ASN:ND2	1:P:165:SER:HB3	2.34	0.41	
1:R:15:ARG:HD3	1:R:15:ARG:HA	1.28	0.41	
1:A:382:LEU:HG	1:A:391:ASP:HB3	2.02	0.41	
1:B:42:PRO:HD3	1:B:82:ASP:OD1	2.19	0.41	
1:B:244:ARG:NH1	1:B:244:ARG:HG3	2.35	0.41	
1:B:478:LEU:HD22	1:B:479:GLU:H	1.85	0.41	
1:G:349:ASP:N	1:G:349:ASP:OD1	2.53	0.41	
1:H:4:LYS:HG3	1:H:78:ASP:OD2	2.21	0.41	
1:L:218:ASN:HB2	1:L:247:MET:HE2	2.03	0.41	
1:M:389:LEU:O	1:M:392:ILE:HB	2.20	0.41	
1:O:293:ILE:N	1:O:294:PRO:HD2	2.35	0.41	
1:P:44:PHE:HB3	1:P:56:THR:O	2.20	0.41	
1:P:400:GLU:O	1:P:404:GLN:HG2	2.21	0.41	
1:R:120:ILE:HG22	1:R:125:MET:HG2	2.02	0.41	
1:B:22:ASP:HB3	1:B:399:LEU:HD21	2.03	0.41	
1:D:286:ASP:OD1	1:D:369:TYR:HB3	2.20	0.41	
1:E:256:PRO:HG2	1:E:296:VAL:HB	2.02	0.41	
1:F:10:ILE:HD11	1:F:367:GLN:HB3	2.02	0.41	
1:F:272:ASN:O	1:F:276:MET:HG2	2.20	0.41	
1:H:142:LEU:HD12	1:H:146:THR:HB	2.02	0.41	
1:I:130:ILE:HG13	1:I:323:ARG:HH22	1.85	0.41	
1:I:215:ASP:O	1:I:219:GLN:HG2	2.20	0.41	
1:K:9:LEU:HD13	1:K:373:LEU:HD22	2.02	0.41	
1:K:339:CYS:SG	1:K:344:ALA:HB2	2.60	0.41	
1:K:464:LYS:HE3	1:K:477:HIS:CE1	2.55	0.41	
1:L:80:CYS:HA	1:L:186:LEU:O	2.20	0.41	
1:O:228:CYS:HB2	1:O:247:MET:HG2	2.03	0.41	
1:R:235:HIS:HA	2:R:507:HOH:O	2.20	0.41	
1:A:272:ASN:O	1:A:276:MET:HG2	2.21	0.41	



	. I		Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:258:LEU:HA	G:258:LEU:HA 1:G:258:LEU:HD23		0.41	
1:G:375:ALA:HB3	1:G:408:LYS:NZ	2.35	0.41	
1:J:293:ILE:O	1:J:296:VAL:HG12	2.20	0.41	
1:L:285:LEU:HB2	1:L:356:ARG:NH1	2.35	0.41	
1:M:141:THR:HG21	1:M:147:LYS:HE2	2.02	0.41	
1:O:210:VAL:HA	1:O:213:ILE:HD12	2.03	0.41	
1:R:82:ASP:HA	1:R:188:ARG:HB3	2.03	0.41	
1:R:312:ILE:HG21	1:R:337:LEU:HD13	2.01	0.41	
1:R:348:ASN:HB3	1:R:351:ALA:HB3	2.03	0.41	
1:C:141:THR:HG23	1:C:147:LYS:HD2	2.01	0.41	
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.94	0.41	
1:E:400:GLU:HG3	1:E:401:GLU:N	2.33	0.41	
1:F:277:CYS:HB2	1:F:281:MET:HE1	2.02	0.41	
1:I:3:LEU:HD11	1:I:186:LEU:HD13	2.01	0.41	
1:M:476:ARG:HE	1:M:476:ARG:HB3	1.67	0.41	
1:P:327:ASN:ND2	1:P:330:SER:HB3	2.35	0.41	
1:Q:302:ASP:OD2	1:Q:331:VAL:HG21	2.20	0.41	
1:A:66:THR:HG22	1:A:69:ASP:CG	2.40	0.41	
1:B:400:GLU:CD	1:B:400:GLU:H	2.24	0.41	
1:C:255:PRO:HG2	1:C:256:PRO:HD3	2.02	0.41	
1:F:381:GLU:CD	1:F:381:GLU:H	2.23	0.41	
1:G:63:LYS:H	1:G:63:LYS:HG2	1.75	0.41	
1:G:80:CYS:HB2	1:G:186:LEU:HD23	2.03	0.41	
1:K:255:PRO:HB2	1:K:256:PRO:HD3	2.02	0.41	
1:L:327:ASN:OD1	1:L:330:SER:HB3	2.20	0.41	
1:N:23:LEU:O	1:N:27:VAL:HG23	2.19	0.41	
1:N:67:TRP:CD2	1:N:182:LYS:HD2	2.56	0.41	
1:O:340:THR:HG22	1:O:393:ASN:OD1	2.20	0.41	
1:O:424:TYR:CE2	1:O:452:CYS:HB3	2.55	0.41	
1:P:388:GLU:HB3	1:P:391:ASP:OD2	2.21	0.41	
1:Q:17:GLY:O	2:Q:501:HOH:O	2.22	0.41	
1:R:292:CYS:SG	1:R:294:PRO:HD2	2.61	0.41	
1:R:390:ARG:HH21	1:R:394:ARG:HH22	1.69	0.41	
1:A:125:MET:HA	1:A:128:ILE:HD12	2.03	0.41	
1:A:142:LEU:HD12	1:A:146:THR:OG1	2.21	0.41	
1:G:87:HIS:CD2	1:G:158:GLN:HG2	2.55	0.41	
1:N:112:VAL:HG13	1:N:151:TRP:HB3	2.02	0.41	
1:P:61:ASP:O	1:P:64:VAL:HG22	2.21	0.41	
1:P:180:THR:HG21	1:P:224:HIS:CB	2.51	0.41	
1:Q:331:VAL:HG23	1:Q:332:GLY:H	1.85	0.41	
1:Q:382:LEU:HA	1:Q:385:GLN:CD	2.41	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:424:TYR:HA	:424:TYR:HA 1:B:425:PRO:HD3		0.41	
1:C:53:SER:O	1:C:89:SER:HB2	2.21	0.41	
1:D:112:VAL:HG22	1:D:162:ASN:HB2	2.03	0.41	
1:G:47:ASN:ND2	1:G:91:GLU:HB2	2.35	0.41	
1:H:4:LYS:HG3	1:H:4:LYS:H	1.70	0.41	
1:H:244:ARG:HH11	1:H:244:ARG:HD3	1.63	0.41	
1:I:222:LEU:HD12	1:I:222:LEU:HA	1.83	0.41	
1:J:113:HIS:HB3	2:J:553:HOH:O	2.20	0.41	
1:J:219:GLN:HG3	1:J:220:VAL:N	2.34	0.41	
1:J:340:THR:HG22	1:J:393:ASN:OD1	2.20	0.41	
1:J:466:THR:HA	1:J:476:ARG:O	2.21	0.41	
1:M:141:THR:HG22	1:M:147:LYS:HE2	2.02	0.41	
1:M:286:ASP:OD2	1:M:369:TYR:HB3	2.20	0.41	
1:N:67:TRP:HZ3	1:N:70:ILE:HG21	1.85	0.41	
1:N:153:THR:HG21	1:N:194:TYR:CD1	2.56	0.41	
1:N:392:ILE:HG12	1:N:393:ASN:N	2.32	0.41	
1:N:400:GLU:CD	1:N:400:GLU:H	2.24	0.41	
1:O:9:LEU:HD13	1:O:373:LEU:HD22	2.02	0.41	
1:O:327:ASN:HD22	1:O:330:SER:HB2	1.86	0.41	
1:P:67:TRP:CE3	1:P:182:LYS:HG3	2.55	0.41	
1:P:130:ILE:O	1:P:323:ARG:NH2	2.50	0.41	
1:Q:97:ASP:HB3	1:Q:107:TYR:HD2	1.86	0.41	
1:R:49:ASP:HB3	1:R:52:PHE:HB2	2.03	0.41	
1:R:388:GLU:HG3	1:R:391:ASP:H	1.86	0.41	
1:R:415:LEU:HD23	1:R:415:LEU:HA	1.93	0.41	
1:A:10:ILE:HG12	1:A:369:TYR:CD1	2.51	0.41	
1:E:75:ALA:HB1	1:N:220:VAL:HA	2.03	0.41	
1:F:39:HIS:HA	1:F:80:CYS:O	2.20	0.41	
1:F:144:ASP:OD1	1:F:146:THR:OG1	2.31	0.41	
1:F:267:SER:O	1:F:271:LYS:HG3	2.21	0.41	
1:F:383:MET:CE	1:F:392:ILE:HB	2.51	0.41	
1:H:130:ILE:O	1:H:130:ILE:HD12	2.20	0.41	
1:H:323:ARG:HE	1:H:323:ARG:HB3	1.68	0.41	
1:K:219:GLN:O	1:K:223:LYS:HG2	2.21	0.41	
1:M:383:MET:HG3	1:M:388:GLU:O	2.20	0.41	
1:N:479:GLU:H	1:N:479:GLU:HG2	1.39	0.41	
1:O:58:LYS:HD3	1:O:178:PHE:CD2	2.56	0.41	
1:O:83:LEU:HG	1:0:172:MET:HE1	2.03	0.41	
1:R:216:TRP:CH2	1:R:220:VAL:HG21	2.56	0.41	
1:R:391:ASP:HA	1:R:394:ARG:CG	2.51	0.41	
1:R:450:TYR:CE2	1:R:470:VAL:HG13	2.55	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:214:LEU:HD12	214:LEU:HD12 1:B:214:LEU:HA		0.40	
1:D:480:CYS:HB2	2:D:572:HOH:O	2.21	0.40	
1:F:213:ILE:O	1:F:217:VAL:HG13	2.21	0.40	
1:H:82:ASP:OD2	1:H:188:ARG:HD3	2.21	0.40	
1:H:140:VAL:HA	2:H:531:HOH:O	2.21	0.40	
1:I:124:ASP:OD2	2:I:502:HOH:O	2.21	0.40	
1:K:55:LEU:O	2:K:502:HOH:O	2.22	0.40	
1:K:285:LEU:HD12	1:K:285:LEU:HA	1.94	0.40	
1:L:100:ALA:HA	1:L:143:SER:HB2	2.04	0.40	
1:N:134:LYS:HG2	1:N:135:GLU:O	2.21	0.40	
1:O:99:ILE:HD11	1:O:140:VAL:CG1	2.51	0.40	
1:P:134:LYS:HB3	1:P:134:LYS:HE2	1.56	0.40	
1:P:258:LEU:HD22	1:P:262:LEU:HD11	2.02	0.40	
1:Q:303:GLU:H	1:Q:303:GLU:HG3	1.61	0.40	
1:R:229:LEU:HD21	1:R:250:TYR:CZ	2.54	0.40	
1:R:454:LEU:HD11	1:R:456:VAL:HG23	2.04	0.40	
1:B:306:LYS:HG3	1:B:331:VAL:HG12	2.02	0.40	
1:D:117:PHE:HB3	1:D:199:ILE:HG13	2.03	0.40	
1:F:328:ILE:H	1:F:328:ILE:HG13	1.54	0.40	
1:G:79:LEU:HD12	1:G:79:LEU:HA	1.89	0.40	
1:G:349:ASP:OD2	1:G:410:VAL:HB	2.20	0.40	
1:G:350:ASP:HB3	1:G:461:LYS:O	2.21	0.40	
1:K:90:ASP:N	1:K:157:GLN:O	2.52	0.40	
1:K:180:THR:HG21	1:K:224:HIS:HB3	2.03	0.40	
1:L:108:ALA:O	1:L:113:HIS:HE1	2.04	0.40	
1:L:134:LYS:H	1:L:134:LYS:HG2	1.63	0.40	
1:L:244:ARG:HG3	1:L:244:ARG:NH1	2.35	0.40	
1:L:272:ASN:O	1:L:276:MET:HG2	2.22	0.40	
1:L:431:PHE:HB2	1:L:445:TRP:CZ2	2.56	0.40	
1:M:2:LEU:HD13	1:M:227:GLU:OE2	2.21	0.40	
1:Q:383:MET:HG3	1:Q:388:GLU:O	2.21	0.40	
1:Q:404:GLN:HG2	1:Q:404:GLN:H	1.60	0.40	
1:C:249:PRO:HG2	1:C:281:MET:HB2	2.03	0.40	
1:C:471:GLU:H	1:C:471:GLU:HG3	1.47	0.40	
1:E:81:VAL:HG21	1:E:179:LEU:HD22	2.04	0.40	
1:F:300:LEU:HD23	1:F:300:LEU:HA	1.92	0.40	
1:G:285:LEU:HD23	1:G:285:LEU:HA	1.86	0.40	
1:I:242:ILE:HG23	1:I:247:MET:HB2	2.03	0.40	
1:I:456:VAL:HG22	1:I:463:VAL:HG22	2.03	0.40	
1:I:469:ASP:HB3	1:I:473:GLY:H	1.86	0.40	
1:J:426:ALA:HA	1:J:447:HIS:HB3	2.03	0.40	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:K:285:LEU:HD21	1:K:355:ALA:HB1	2.04	0.40	
1:N:90:ASP:HB3	1:N:159:ILE:HD11	2.04	0.40	
1:N:214:LEU:HD23	1:N:214:LEU:HA	1.93	0.40	
1:N:242:ILE:HG23	1:N:247:MET:HB2	2.03	0.40	
1:0:15:ARG:HD2	1:O:396:TYR:CD2	2.57	0.40	
1:P:346:MET:HE3	1:P:346:MET:HB2	1.93	0.40	
1:R:286:ASP:HB3	1:R:341:PHE:HB2	2.03	0.40	
1:R:380:HIS:HA	1:R:392:ILE:CD1	2.52	0.40	
1:C:380:HIS:CE1	1:C:392:ILE:HD11	2.57	0.40	
1:D:230:PRO:HG3	1:D:247:MET:HE1	2.02	0.40	
1:F:182:LYS:HA	1:F:182:LYS:HD2	1.77	0.40	
1:G:223:LYS:HG3	1:G:224:HIS:N	2.36	0.40	
1:G:356:ARG:NH1	1:G:368:VAL:HG22	2.37	0.40	
1:J:86:ASN:HB3	1:J:87:HIS:ND1	2.36	0.40	
1:K:380:HIS:O	1:K:384:GLU:HG2	2.21	0.40	
1:0:123:ASP:0	1:O:127:LYS:HG3	2.22	0.40	
1:O:397:TYR:HA	1:O:401:GLU:OE1	2.21	0.40	
1:P:12:TYR:CZ	1:P:41:LEU:HD22	2.56	0.40	
1:P:390:ARG:HB3	1:P:394:ARG:HD2	2.03	0.40	
1:Q:413:ARG:NH2	1:Q:480:CYS:OXT	2.46	0.40	
1:B:12:TYR:CG	1:B:15:ARG:HG2	2.56	0.40	
1:B:192:PHE:HE2	1:B:232:VAL:HG22	1.85	0.40	
1:B:461:LYS:NZ	1:G:133:GLU:OE1	2.52	0.40	
1:H:76:LYS:HB2	1:H:76:LYS:HE2	1.86	0.40	
1:I:80:CYS:HA	1:I:186:LEU:O	2.21	0.40	
1:K:322:ARG:HG3	1:K:332:GLY:O	2.21	0.40	
1:M:138:ARG:NH1	1:M:156:GLU:O	2.54	0.40	
1:M:441:VAL:HG22	1:M:456:VAL:HB	2.04	0.40	
1:O:41:LEU:HD13	1:O:41:LEU:HA	1.89	0.40	
1:O:308:LEU:O	1:O:312:ILE:HG12	2.21	0.40	
1:P:325:ALA:CB	1:P:333:ALA:HA	2.51	0.40	
1:P:471:GLU:H	1:P:471:GLU:HG3	1.54	0.40	
1:Q:15:ARG:HD3	1:Q:396:TYR:CE2	2.56	0.40	
1:Q:402:VAL:O	1:Q:406:ILE:HG12	2.22	0.40	
1:R:22:ASP:O	1:R:26:VAL:HG13	2.20	0.40	
1:R:131:ARG:HD3	1:R:322:ARG:HA	2.03	0.40	

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	478/480~(100%)	465~(97%)	13 (3%)	0	100	100
1	В	478/480~(100%)	464 (97%)	14 (3%)	0	100	100
1	С	478/480~(100%)	468~(98%)	10 (2%)	0	100	100
1	D	478/480~(100%)	469~(98%)	9(2%)	0	100	100
1	Е	477/480~(99%)	464~(97%)	13 (3%)	0	100	100
1	F	478/480~(100%)	464 (97%)	14 (3%)	0	100	100
1	G	477/480~(99%)	463~(97%)	14 (3%)	0	100	100
1	Н	478/480~(100%)	466~(98%)	12 (2%)	0	100	100
1	Ι	478/480~(100%)	467~(98%)	11 (2%)	0	100	100
1	J	478/480~(100%)	462~(97%)	16 (3%)	0	100	100
1	Κ	478/480~(100%)	468~(98%)	10 (2%)	0	100	100
1	L	478/480~(100%)	467~(98%)	11 (2%)	0	100	100
1	М	478/480~(100%)	462~(97%)	16 (3%)	0	100	100
1	Ν	478/480~(100%)	465~(97%)	13 (3%)	0	100	100
1	Ο	478/480~(100%)	467~(98%)	11 (2%)	0	100	100
1	Р	478/480~(100%)	466~(98%)	12 (2%)	0	100	100
1	Q	478/480~(100%)	463~(97%)	15(3%)	0	100	100
1	R	478/480~(100%)	466 (98%)	12 (2%)	0	100	100
All	All	8602/8640 (100%)	8376 (97%)	226 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	426/426~(100%)	409 (96%)	17 (4%)	31 49
1	В	426/426~(100%)	401 (94%)	25~(6%)	19 32
1	С	426/426~(100%)	402 (94%)	24 (6%)	21 34
1	D	426/426~(100%)	402 (94%)	24 (6%)	21 34
1	Е	425/426~(100%)	404 (95%)	21 (5%)	25 40
1	F	424/426~(100%)	402 (95%)	22 (5%)	23 38
1	G	425/426~(100%)	388 (91%)	37 (9%)	10 15
1	Н	426/426~(100%)	395~(93%)	31 (7%)	14 22
1	Ι	426/426~(100%)	395~(93%)	31 (7%)	14 22
1	J	426/426~(100%)	391 (92%)	35 (8%)	11 17
1	Κ	426/426~(100%)	390~(92%)	36 (8%)	10 16
1	L	426/426~(100%)	375~(88%)	51 (12%)	5 6
1	М	426/426~(100%)	381 (89%)	45 (11%)	6 9
1	Ν	426/426~(100%)	388~(91%)	38 (9%)	9 14
1	Ο	426/426~(100%)	393~(92%)	33 (8%)	13 20
1	Р	426/426~(100%)	382~(90%)	44 (10%)	7 10
1	Q	426/426~(100%)	397~(93%)	29 (7%)	16 25
1	R	426/426~(100%)	379~(89%)	47 (11%)	6 8
All	All	7664/7668~(100%)	7074 (92%)	590 (8%)	13 20

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

All (590) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	А	10	ILE
1	А	15	ARG
1	А	18	ASN
1	А	41	LEU
1	А	119	GLU
1	А	152	CYS
1	А	232	VAL
1	А	281	MET
1	А	324	SER
1	А	388	GLU



Mol	Chain	Res	Type
1	А	390	ARG
1	А	416	SER
1	А	439	SER
1	А	471	GLU
1	А	476	ARG
1	А	479	GLU
1	В	1	MET
1	В	2	LEU
1	В	15	ARG
1	В	69	ASP
1	В	109	ASP
1	В	131	ARG
1	В	152	CYS
1	В	166	ASP
1	В	196	THR
1	В	214	LEU
1	В	231	GLU
1	В	232	VAL
1	В	245	ARG
1	В	250	TYR
1	В	279	ARG
1	В	304	LYS
1	В	327	ASN
1	В	339	CYS
1	В	384	GLU
1	В	385	GLN
1	В	471	GLU
1	В	472	THR
1	В	478	LEU
1	В	479	GLU
1	В	480	CYS
1	С	15	ARG
1	С	41	LEU
1	С	76	LYS
1	С	105	SER
1	C	152	CYS
1	С	182	LYS
1	С	223	LYS
1	С	236	THR
1	С	279	ARG
1	C	280	ASN
1	С	281	MET



Mol	Chain	Res	Type
1	С	338	THR
1	С	343	ASP
1	С	381	GLU
1	С	383	MET
1	С	416	SER
1	С	439	SER
1	С	469	ASP
1	С	471	GLU
1	С	474	GLU
1	С	476	ARG
1	С	477	HIS
1	С	478	LEU
1	С	480	CYS
1	D	15	ARG
1	D	41	LEU
1	D	76	LYS
1	D	131	ARG
1	D	138	ARG
1	D	165	SER
1	D	181	SER
1	D	232	VAL
1	D	243	SER
1	D	244	ARG
1	D	258	LEU
1	D	279	ARG
1	D	281	MET
1	D	302	ASP
1	D	338	THR
1	D	343	ASP
1	D	374	LEU
1	D	381	GLU
1	D	385	GLN
1	D	407	GLN
1	D	408	LYS
1	D	416	SER
1	D	471	GLU
1	D	476	ARG
1	E	15	ARG
1	E	39	HIS
1	Е	76	LYS
1	E	131	ARG
1	Е	134	LYS



Mol	Chain	Res	Type
1	Е	139	GLU
1	Е	140	VAL
1	Е	144	ASP
1	Е	148	THR
1	Е	152	CYS
1	Е	222	LEU
1	Е	234	ASP
1	Е	279	ARG
1	Е	281	MET
1	Е	308	LEU
1	Е	385	GLN
1	Е	386	SER
1	Е	400	GLU
1	Е	403	GLU
1	Ε	404	GLN
1	Е	439	SER
1	F	41	LEU
1	F	76	LYS
1	F	119	GLU
1	F	130	ILE
1	F	131	ARG
1	F	132	LYS
1	F	134	LYS
1	F	144	ASP
1	F	166	ASP
1	F	185	ASN
1	F	215	ASP
1	F	217	VAL
1	F	250	TYR
1	F	279	ARG
1	F	302	ASP
1	F	303	GLU
1	F	304	LYS
1	F	306	LYS
1	F	385	GLN
1	F	390	ARG
1	F	416	SER
1	F	479	GLU
1	G	41	LEU
1	G	71	GLU
1	G	89	SER
1	G	116	LYS



Mol	Chain	Res	Type
1	G	121	SER
1	G	123	ASP
1	G	140	VAL
1	G	147	LYS
1	G	148	THR
1	G	184	VAL
1	G	185	ASN
1	G	219	GLN
1	G	222	LEU
1	G	223	LYS
1	G	227	GLU
1	G	232	VAL
1	G	236	THR
1	G	279	ARG
1	G	281	MET
1	G	302	ASP
1	G	304	LYS
1	G	330	SER
1	G	343	ASP
1	G	349	ASP
1	G	383	MET
1	G	392	ILE
1	G	400	GLU
1	G	408	LYS
1	G	417	LEU
1	G	419	LYS
1	G	439	SER
1	G	441	VAL
1	G	449	ASP
1	G	470	VAL
1	G	476	ARG
1	G	478	LEU
1	G	479	GLU
1	H	15	ARG
1	Н	30	HIS
1	Н	38	LEU
1	Н	39	HIS
1	Н	76	LYS
1	Н	109	ASP
1	Н	116	LYS
1	H	133	GLU
1	Н	147	LYS



Mol	Chain	Res	Type
1	Н	152	CYS
1	Н	174	SER
1	Н	231	GLU
1	Н	279	ARG
1	Н	280	ASN
1	Н	303	GLU
1	Н	322	ARG
1	Н	324	SER
1	Н	331	VAL
1	Н	343	ASP
1	Н	383	MET
1	Н	385	GLN
1	Н	390	ARG
1	Н	392	ILE
1	Н	400	GLU
1	Н	407	GLN
1	Н	408	LYS
1	Н	439	SER
1	Н	464	LYS
1	Н	470	VAL
1	Н	471	GLU
1	Н	472	THR
1	Ι	76	LYS
1	Ι	89	SER
1	Ι	115	ASP
1	Ι	133	GLU
1	Ι	134	LYS
1	Ι	142	LEU
1	Ι	152	CYS
1	Ι	154	PHE
1	Ι	160	ASP
1	Ι	165	SER
1	Ι	166	ASP
1	Ι	190	ASP
1	Ι	215	ASP
1	Ι	222	LEU
1	Ι	223	LYS
1	Ι	236	THR
1	Ι	244	ARG
1	Ι	245	ARG
1	Ι	247	MET
1	Ι	250	TYR



Mol	Chain	Res	Type
1	Ι	302	ASP
1	Ι	303	GLU
1	Ι	321	MET
1	Ι	323	ARG
1	Ι	381	GLU
1	Ι	383	MET
1	Ι	389	LEU
1	Ι	392	ILE
1	Ι	400	GLU
1	Ι	464	LYS
1	Ι	478	LEU
1	J	21	LYS
1	J	41	LEU
1	J	68	ASP
1	J	76	LYS
1	J	101	ASN
1	J	105	SER
1	J	121	SER
1	J	133	GLU
1	J	134	LYS
1	J	184	VAL
1	J	196	THR
1	J	219	GLN
1	J	231	GLU
1	J	234	ASP
1	J	245	ARG
1	J	279	ARG
1	J	280	ASN
1	J	281	MET
1	J	302	ASP
1	J	304	LYS
1	J	330	SER
1	J	343	ASP
1	J	374	LEU
1	J	381	GLU
1	J	384	GLU
1	J	388	GLU
1	J	391	ASP
1	J	400	GLU
1	J	415	LEU
1	J	416	SER
1	J	439	SER



Mol	Chain	Res	Type
1	J	471	GLU
1	J	476	ARG
1	J	478	LEU
1	J	480	CYS
1	K	25	THR
1	K	28	ASP
1	K	38	LEU
1	К	74	THR
1	K	92	SER
1	K	109	ASP
1	К	115	ASP
1	K	127	LYS
1	Κ	129	HIS
1	K	131	ARG
1	К	133	GLU
1	K	140	VAL
1	K	147	LYS
1	K	149	ARG
1	K	152	CYS
1	K	174	SER
1	K	184	VAL
1	K	219	GLN
1	K	222	LEU
1	K	224	HIS
1	K	250	TYR
1	K	279	ARG
1	K	281	MET
1	K	302	ASP
1	K	306	LYS
1	K	322	ARG
1	K	323	ARG
1	K	330	SER
1	K	343	ASP
1	K	374	LEU
1	K	381	GLU
1	K	383	MET
1	K	385	GLN
1	K	390	ARG
1	K	439	SER
1	K	464	LYS
1	L	1	MET
1	L	15	ARG



Mol	Chain	Res	Type
1	L	33	GLU
1	L	38	LEU
1	L	41	LEU
1	L	63	LYS
1	L	66	THR
1	L	71	GLU
1	L	76	LYS
1	L	82	ASP
1	L	84	THR
1	L	105	SER
1	L	106	GLU
1	L	109	ASP
1	L	119	GLU
1	L	121	SER
1	L	128	ILE
1	L	131	ARG
1	L	134	LYS
1	L	143	SER
1	L	147	LYS
1	L	149	ARG
1	L	160	ASP
1	L	165	SER
1	L	174	SER
1	L	184	VAL
1	L	185	ASN
1	L	219	GLN
1	L	222	LEU
1	L	223	LYS
1	L	234	ASP
1	L	279	ARG
1	L	280	ASN
1	L	281	MET
1	L	302	ASP
1	L	321	MET
1	L	322	ARG
1	L	323	ARG
1	L	381	GLU
1	L	383	MET
1	L	388	GLU
1	L	392	ILE
1	L	398	THR
1	L	400	GLU



Mol	Chain	Res	Type
1	L	406	ILE
1	L	430	HIS
1	L	432	GLU
1	L	439	SER
1	L	468	THR
1	L	471	GLU
1	L	479	GLU
1	М	1	MET
1	М	31	LEU
1	М	32	SER
1	М	39	HIS
1	М	41	LEU
1	М	63	LYS
1	М	71	GLU
1	М	76	LYS
1	М	89	SER
1	М	130	ILE
1	М	131	ARG
1	М	133	GLU
1	М	140	VAL
1	М	152	CYS
1	М	166	ASP
1	М	173	GLU
1	М	190	ASP
1	М	196	THR
1	М	232	VAL
1	М	243	SER
1	М	244	ARG
1	М	250	TYR
1	М	280	ASN
1	М	281	MET
1	М	287	THR
1	М	296	VAL
1	М	302	ASP
1	М	315	ARG
1	М	321	MET
1	М	322	ARG
1	М	330	SER
1	М	338	THR
1	М	385	GLN
1	М	390	ARG
1	М	392	ILE



Mol	Chain	Res	Type
1	М	398	THR
1	М	400	GLU
1	М	404	GLN
1	М	408	LYS
1	М	439	SER
1	М	449	ASP
1	М	471	GLU
1	М	474	GLU
1	М	476	ARG
1	М	480	CYS
1	Ν	15	ARG
1	Ν	41	LEU
1	N	47	ASN
1	N	59	GLU
1	Ν	69	ASP
1	Ν	76	LYS
1	N	80	CYS
1	N	89	SER
1	N	105	SER
1	Ν	109	ASP
1	N	130	ILE
1	N	131	ARG
1	N	133	GLU
1	N	134	LYS
1	N	136	PRO
1	N	137	PHE
1	N	138	ARG
1	N	139	GLU
1	N	154	PHE
1	Ν	180	THR
1	N	231	GLU
1	N	245	ARG
1	N	279	ARG
1	N	302	ASP
1	N	303	GLU
1	N	306	LYS
1	N	324	SER
1	N	343	ASP
1	N	390	ARG
1	N	392	ILE
1	N	398	THR
1	Ν	401	GLU



Mol	Chain	Res	Type
1	N	404	GLN
1	N	408	LYS
1	N	449	ASP
1	Ν	466	THR
1	Ν	479	GLU
1	Ν	480	CYS
1	0	14	ASP
1	0	15	ARG
1	0	21	LYS
1	0	41	LEU
1	0	69	ASP
1	0	70	ILE
1	0	76	LYS
1	0	96	THR
1	0	105	SER
1	0	134	LYS
1	0	137	PHE
1	0	155	THR
1	0	165	SER
1	0	196	THR
1	0	201	THR
1	0	247	MET
1	0	250	TYR
1	0	280	ASN
1	0	281	MET
1	0	313	ASP
1	0	315	ARG
1	0	322	ARG
1	0	381	GLU
1	Ο	384	GLU
1	0	388	GLU
1	0	391	ASP
1	0	398	THR
1	0	404	GLN
1	0	439	SER
1	0	441	VAL
1	0	471	GLU
1	0	476	ARG
1	0	479	GLU
1	P	1	MET
1	P	4	LYS
1	Р	28	ASP



Mol	Chain	Res	Type
1	Р	76	LYS
1	Р	81	VAL
1	Р	109	ASP
1	Р	112	VAL
1	Р	115	ASP
1	Р	123	ASP
1	Р	132	LYS
1	Р	134	LYS
1	Р	139	GLU
1	Р	144	ASP
1	Р	146	THR
1	Р	147	LYS
1	Р	148	THR
1	Р	149	ARG
1	Р	165	SER
1	Р	167	LEU
1	Р	182	LYS
1	Р	222	LEU
1	Р	245	ARG
1	Р	258	LEU
1	Р	279	ARG
1	Р	280	ASN
1	Р	302	ASP
1	Р	318	ASP
1	Р	322	ARG
1	Р	323	ARG
1	Р	378	ASN
1	Р	382	LEU
1	Р	383	MET
1	Р	385	GLN
1	Р	390	ARG
1	Р	392	ILE
1	Р	398	THR
1	Р	416	SER
1	Р	419	LYS
1	Р	439	SER
1	Р	449	ASP
1	Р	464	LYS
1	Р	475	THR
1	Р	476	ARG
1	Р	479	GLU
1	Q	9	LEU



Mol	Chain	Res	Type
1	Q	41	LEU
1	Q	76	LYS
1	Q	106	GLU
1	Q	119	GLU
1	Q	140	VAL
1	Q	144	ASP
1	Q	152	CYS
1	Q	185	ASN
1	Q	188	ARG
1	Q	227	GLU
1	Q	231	GLU
1	Q	236	THR
1	Q	250	TYR
1	Q	264	ASP
1	Q	302	ASP
1	Q	303	GLU
1	Q	315	ARG
1	Q	323	ARG
1	Q	324	SER
1	Q	385	GLN
1	Q	389	LEU
1	Q	390	ARG
1	Q	400	GLU
1	Q	404	GLN
1	Q	474	GLU
1	Q	476	ARG
1	Q	479	GLU
1	Q	480	CYS
1	R	15	ARG
1	R	23	LEU
1	R	28	ASP
1	R	39	HIS
1	R	40	ILE
1	R	56	THR
1	R	63	LYS
1	R	66	THR
1	R	67	TRP
1	R	76	LYS
1	R	79	LEU
1	R	82	ASP
1	R	89	SER
1	R	109	ASP



Mol	Chain	Res	Type
1	R	131	ARG
1	R	132	LYS
1	R	133	GLU
1	R	138	ARG
1	R	152	CYS
1	R	156	GLU
1	R	161	LEU
1	R	165	SER
1	R	174	SER
1	R	190	ASP
1	R	224	HIS
1	R	231	GLU
1	R	236	THR
1	R	244	ARG
1	R	250	TYR
1	R	279	ARG
1	R	296	VAL
1	R	313	ASP
1	R	322	ARG
1	R	328	ILE
1	R	329	HIS
1	R	330	SER
1	R	343	ASP
1	R	381	GLU
1	R	385	GLN
1	R	391	ASP
1	R	399	LEU
1	R	407	GLN
1	R	408	LYS
1	R	464	LYS
1	R	472	THR
1	R	474	GLU
1	R	476	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	404	GLN
1	В	39	HIS
1	В	218	ASN
1	В	224	HIS
1	В	327	ASN



Mol	Chain	Res	Type
1	С	219	GLN
1	D	385	GLN
1	D	412	GLN
1	D	430	HIS
1	D	453	HIS
1	Е	39	HIS
1	Е	162	ASN
1	Е	280	ASN
1	F	129	HIS
1	F	329	HIS
1	F	347	GLN
1	F	385	GLN
1	G	129	HIS
1	G	157	GLN
1	Н	18	ASN
1	Н	129	HIS
1	Н	412	GLN
1	Ι	87	HIS
1	Ι	129	HIS
1	Ι	239	GLN
1	J	30	HIS
1	J	47	ASN
1	J	57	HIS
1	J	423	ASN
1	K	219	GLN
1	К	224	HIS
1	K	233	HIS
1	K	385	GLN
1	K	430	HIS
1	L	219	GLN
1	L	380	HIS
1	L	385	GLN
1	L	404	GLN
1	М	219	GLN
1	М	224	HIS
1	М	385	GLN
1	М	395	HIS
1	М	407	GLN
1	Ν	30	HIS
1	N	404	GLN
1	0	404	GLN
1	Р	280	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	Р	385	GLN
1	R	157	GLN
1	R	224	HIS
1	R	280	ASN
1	R	347	GLN
1	R	459	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	$OWAB(A^2)$	Q<0.9
1	А	480/480~(100%)	-0.08	10 (2%) 63 61	26, 38, 59, 87	0
1	В	480/480 (100%)	0.02	8 (1%) 70 68	26, 41, 61, 97	0
1	С	480/480~(100%)	-0.19	8 (1%) 70 68	29, 38, 55, 97	0
1	D	480/480~(100%)	-0.07	9 (1%) 66 64	29, 44, 60, 86	0
1	Ε	479/480~(99%)	-0.04	13 (2%) 54 52	26, 39, 64, 91	0
1	F	480/480~(100%)	0.05	9 (1%) 66 64	32, 46, 68, 94	0
1	G	479/480~(99%)	0.03	10 (2%) 63 61	29, 43, 71, 98	0
1	Н	480/480 (100%)	0.19	21 (4%) 34 33	26, 44, 71, 87	0
1	Ι	480/480 (100%)	0.14	15 (3%) 49 47	32, 49, 72, 92	0
1	J	480/480 (100%)	0.11	18 (3%) 40 39	36, 48, 69, 93	0
1	K	480/480 (100%)	0.16	11 (2%) 60 58	28, 48, 65, 82	0
1	L	480/480 (100%)	0.28	25 (5%) 27 26	32, 50, 75, 90	0
1	М	480/480 (100%)	0.25	17 (3%) 44 43	34, 48, 70, 111	0
1	Ν	480/480 (100%)	0.43	32 (6%) 17 16	29, 52, 81, 105	0
1	Ο	480/480~(100%)	0.38	31 (6%) 18 17	39, 57, 79, 103	0
1	Р	480/480~(100%)	0.78	52 (10%) 5 5	37, 64, 96, 112	0
1	Q	480/480 (100%)	0.20	20 (4%) 36 35	39, 51, 71, 100	0
1	R	480/480 (100%)	0.38	23 (4%) 30 29	30, 55, 79, 116	0
All	All	8638/8640 (99%)	0.17	332 (3%) 40 39	26, 47, 74, 116	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Р	470	VAL	7.6
1	Н	142	LEU	6.4
1	Р	480	CYS	6.3



Mol	Chain	Res	Type	RSRZ
1	Е	480	CYS	6.2
1	0	479	GLU	6.1
1	Ν	104	ASP	5.9
1	Р	478	LEU	5.6
1	Р	146	THR	5.6
1	Ν	142	LEU	5.5
1	Ν	141	THR	5.3
1	С	470	VAL	5.3
1	Р	104	ASP	5.2
1	Ν	143	SER	5.1
1	Р	148	THR	5.0
1	М	470	VAL	5.0
1	Н	143	SER	4.9
1	J	472	THR	4.9
1	Ν	140	VAL	4.8
1	Р	474	GLU	4.8
1	Е	470	VAL	4.6
1	М	480	CYS	4.6
1	D	479	GLU	4.6
1	D	471	GLU	4.5
1	С	471	GLU	4.5
1	L	479	GLU	4.5
1	Н	144	ASP	4.5
1	Ν	480	CYS	4.4
1	В	470	VAL	4.4
1	G	470	VAL	4.4
1	R	470	VAL	4.4
1	Q	473	GLY	4.3
1	Q	470	VAL	4.3
1	J	473	GLY	4.2
1	L	324	SER	4.2
1	Н	470	VAL	4.2
1	С	472	THR	4.2
1	R	473	GLY	4.2
1	Н	103	PHE	4.2
1	N	100	ALA	4.2
1	Q	480	CYS	4.2
1	G	471	GLU	4.1
1	А	476	ARG	4.1
1	Q	479	GLU	4.1
1	Р	467	TYR	4.0
1	Р	471	GLU	4.0



Mol	Chain	Res	Type	RSRZ
1	Ο	140	VAL	4.0
1	В	479	GLU	4.0
1	N	108	ALA	3.9
1	В	471	GLU	3.9
1	Ι	480	CYS	3.9
1	R	279	ARG	3.8
1	В	474	GLU	3.8
1	Е	472	THR	3.8
1	Ν	146	THR	3.8
1	Q	474	GLU	3.7
1	Ι	140	VAL	3.7
1	0	480	CYS	3.7
1	0	470	VAL	3.7
1	Q	478	LEU	3.7
1	М	76	LYS	3.7
1	Н	480	CYS	3.7
1	Р	385	GLN	3.7
1	J	470	VAL	3.7
1	Н	98	PHE	3.7
1	L	323	ARG	3.6
1	Н	479	GLU	3.6
1	Е	479	GLU	3.6
1	Р	380	HIS	3.6
1	В	472	THR	3.6
1	Р	96	THR	3.6
1	Н	140	VAL	3.6
1	Р	103	PHE	3.5
1	0	146	THR	3.5
1	Ν	98	PHE	3.5
1	Ν	148	THR	3.5
1	Р	98	PHE	3.5
1	G	479	GLU	3.5
1	Ι	479	GLU	3.5
1	Q	472	THR	3.5
1	L	163	TYR	3.4
1	L	314	ALA	3.4
1	Р	472	THR	3.4
1	С	473	GLY	3.4
1	Q	100	ALA	3.4
1	N	1	MET	3.4
1	М	471	GLU	3.4
1	М	474	GLU	3.4



Mol	Chain	Res	Type	RSRZ
1	Ι	323	ARG	3.4
1	Е	148	THR	3.4
1	Р	469	ASP	3.3
1	Ν	139	GLU	3.3
1	Ν	103	PHE	3.3
1	L	325	ALA	3.3
1	0	472	THR	3.3
1	0	476	ARG	3.3
1	Р	473	GLY	3.3
1	Р	100	ALA	3.3
1	Н	102	GLY	3.3
1	N	387	GLY	3.3
1	Η	471	GLU	3.3
1	Р	378	ASN	3.2
1	Р	479	GLU	3.2
1	J	279	ARG	3.2
1	N	144	ASP	3.2
1	Ι	143	SER	3.2
1	L	322	ARG	3.2
1	0	404	GLN	3.2
1	0	98	PHE	3.2
1	Н	104	ASP	3.2
1	J	468	THR	3.2
1	J	471	GLU	3.2
1	Q	385	GLN	3.1
1	N	407	GLN	3.1
1	А	388	GLU	3.1
1	Е	474	GLU	3.1
1	Р	30	HIS	3.1
1	М	109	ASP	3.1
1	Р	475	THR	3.1
1	L	107	TYR	3.0
1	Р	2	LEU	3.0
1	P	147	LYS	3.0
1	К	279	ARG	3.0
1	Н	108	ALA	3.0
1	Р	142	LEU	3.0
1	М	473	GLY	3.0
1	Е	471	GLU	3.0
1	Q	316	SER	3.0
1	0	109	ASP	2.9
1	Р	137	PHE	2.9



Mol	Chain	Res	Type	RSRZ
1	L	102	GLY	2.9
1	А	480	CYS	2.9
1	G	480	CYS	2.9
1	Ι	139	GLU	2.9
1	0	104	ASP	2.9
1	Р	383	MET	2.9
1	0	385	GLN	2.9
1	N	145	GLY	2.9
1	R	329	HIS	2.9
1	F	471	GLU	2.9
1	J	407	GLN	2.9
1	R	73	PHE	2.9
1	J	475	THR	2.9
1	Q	471	GLU	2.9
1	N	107	TYR	2.9
1	N	329	HIS	2.8
1	L	480	CYS	2.8
1	G	328	ILE	2.8
1	D	473	GLY	2.8
1	R	479	GLU	2.8
1	L	104	ASP	2.8
1	L	145	GLY	2.8
1	R	480	CYS	2.8
1	L	388	GLU	2.8
1	N	99	ILE	2.8
1	F	329	HIS	2.8
1	G	449	ASP	2.8
1	K	407	GLN	2.7
1	L	141	THR	2.7
1	Ο	148	THR	2.7
1	D	478	LEU	2.7
1	Р	167	LEU	2.7
1	Ι	133	GLU	2.7
1	А	474	GLU	2.7
1	F	131	ARG	2.7
1	F	133	GLU	2.7
1	Р	476	ARG	2.7
1	K	314	ALA	2.7
1	F	328	ILE	2.7
1	Н	148	THR	2.7
1	R	450	TYR	2.7
1	Е	277	CYS	2.7



Mol	Chain	Res	Type	RSRZ
1	J	474	GLU	2.7
1	N	479	GLU	2.7
1	Q	106	GLU	2.7
1	Н	146	THR	2.7
1	K	430	HIS	2.7
1	J	476	ARG	2.6
1	L	385	GLN	2.6
1	Q	388	GLU	2.6
1	А	472	THR	2.6
1	Ι	155	THR	2.6
1	G	223	LYS	2.6
1	Р	328	ILE	2.6
1	F	325	ALA	2.6
1	Р	102	GLY	2.6
1	М	472	THR	2.6
1	N	76	LYS	2.6
1	R	382	LEU	2.6
1	Р	384	GLU	2.6
1	N	101	ASN	2.6
1	Ν	147	LYS	2.6
1	F	479	GLU	2.6
1	М	384	GLU	2.6
1	L	386	SER	2.6
1	0	474	GLU	2.6
1	0	383	MET	2.6
1	N	102	GLY	2.5
1	K	148	THR	2.5
1	Q	146	THR	2.5
1	0	473	GLY	2.5
1	J	385	GLN	2.5
1	Н	279	ARG	2.5
1	В	384	GLU	2.5
1	J	477	HIS	2.5
1	D	279	ARG	2.5
1	L	119	GLU	2.5
1	Р	419	LYS	2.5
1	Ι	478	LEU	2.5
1	R	140	VAL	2.5
1	R	142	LEU	2.5
1	А	384	GLU	2.5
1	R	474	GLU	2.5
1	0	216	TRP	2.5



Mol	Chain	Res	Type	RSRZ
1	Е	139	GLU	2.5
1	М	479	GLU	2.5
1	0	407	GLN	2.4
1	Ι	407	GLN	2.4
1	R	314	ALA	2.4
1	Е	104	ASP	2.4
1	J	384	GLU	2.4
1	Р	130	ILE	2.4
1	Н	280	ASN	2.4
1	Ν	323	ARG	2.4
1	Q	405	ASP	2.4
1	L	131	ARG	2.4
1	Р	279	ARG	2.4
1	А	479	GLU	2.4
1	R	35	ILE	2.4
1	G	147	LYS	2.4
1	А	475	THR	2.4
1	В	480	CYS	2.4
1	D	388	GLU	2.4
1	Н	147	LYS	2.4
1	Ι	103	PHE	2.4
1	0	450	TYR	2.4
1	L	381	GLU	2.4
1	Р	31	LEU	2.4
1	Κ	224	HIS	2.3
1	Р	76	LYS	2.3
1	Е	473	GLY	2.3
1	F	313	ASP	2.3
1	N	279	ARG	2.3
1	В	276	MET	2.3
1	Н	141	THR	2.3
1	R	137	PHE	2.3
1	Q	107	TYR	2.3
1	Р	185	ASN	2.3
1	0	471	GLU	2.3
1	М	1	MET	2.3
1	Ι	322	ARG	2.3
1	L	143	SER	2.3
1	Р	317	ALA	2.3
1	Р	450	TYR	2.3
1	L	478	LEU	2.3
1	0	384	GLU	2.3



Mol	Chain	Res	Type	RSRZ
1	А	473	GLY	2.2
1	Ι	404	GLN	2.2
1	R	109	ASP	2.2
1	Р	95	PHE	2.2
1	М	279	ARG	2.2
1	С	469	ASP	2.2
1	R	448	GLY	2.2
1	М	100	ALA	2.2
1	Q	99	ILE	2.2
1	0	103	PHE	2.2
1	С	404	GLN	2.2
1	Ι	107	TYR	2.2
1	0	107	TYR	2.2
1	R	472	THR	2.2
1	Р	139	GLU	2.2
1	Q	101	ASN	2.2
1	Е	146	THR	2.2
1	0	141	THR	2.2
1	L	224	HIS	2.2
1	J	405	ASP	2.2
1	L	148	THR	2.2
1	0	70	ILE	2.2
1	Р	101	ASN	2.2
1	С	479	GLU	2.2
1	J	469	ASP	2.1
1	0	144	ASP	2.1
1	Р	140	VAL	2.1
1	0	280	ASN	2.1
1	K	183	GLY	2.1
1	0	312	ILE	2.1
1	G	279	ARG	2.1
1	М	383	MET	2.1
1	K	331	VAL	2.1
1	R	326	ALA	2.1
1	Ι	99	ILE	2.1
1	Р	159	ILE	2.1
1	М	478	LEU	2.1
1	K	313	ASP	2.1
1	R	104	ASP	2.1
1	J	479	GLU	2.1
1	0	106	GLU	2.1
1	Е	476	ARG	2.1



Mol	Chain	Res	Type	RSRZ
1	Р	166	ASP	2.1
1	Р	391	ASP	2.1
1	Р	132	LYS	2.1
1	L	146	THR	2.1
1	0	110	LEU	2.1
1	0	279	ARG	2.1
1	Q	111	PHE	2.1
1	R	43	PHE	2.1
1	J	381	GLU	2.1
1	С	476	ARG	2.1
1	М	74	THR	2.1
1	D	477	HIS	2.1
1	Ν	115	ASP	2.1
1	Р	449	ASP	2.1
1	Ν	105	SER	2.1
1	А	471	GLU	2.1
1	F	119	GLU	2.1
1	Н	410	VAL	2.1
1	Н	117	PHE	2.1
1	D	480	CYS	2.1
1	М	385	GLN	2.1
1	Р	381	GLU	2.1
1	L	317	ALA	2.0
1	Р	168	ALA	2.0
1	Р	107	TYR	2.0
1	R	328	ILE	2.0
1	Ν	149	ARG	2.0
1	D	472	THR	2.0
1	K	146	THR	2.0
1	J	219	GLN	2.0
1	G	473	GLY	2.0
1	K	384	GLU	2.0
1	Q	383	MET	2.0
1	R	471	GLU	2.0
1	Ν	325	ALA	2.0

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

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


6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

