

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

#### Sep 23, 2024 – 12:21 PM JST

PDB ID	:	8ZQA
Title	:	Crystal structure of 1,4-alpha-glucan branching protein from Rhodothermus
		profundi
Authors	:	Li, Q.; Zong, Z.Y.; Liu, W.D.
Deposited on	:	2024-06-01
Resolution	:	2.91  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
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 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 2.91 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	164625	2797 (2.94-2.90)
Clashscore	180529	3049(2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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	620	2%	210/	
1	A	020	65%	31%	• •
1	В	620	72%	24%	••
1	С	620	<sup>2%</sup> 66%	30%	•••
1	D	620	% 68%	26%	••
1	Е	620	73%	24%	••
1	F	620	<sup>2%</sup> 64%	30%	•••



Mol	Chain	Length	Quality of chain				
1	G	620	<sup>2%</sup> 70%	26%			
1	Н	620	5% 66%	29%	•••		



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 39395 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	Δ	602	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	005	4886	3190	817	865	14	0	0	0
1	В	603	Total	С	Ν	0	S	0	0	0
	D	005	4925	3212	832	867	14	0	0	0
1	C	606	Total	С	Ν	0	S	0	0	0
	U	000	4925	3209	826	875	15	0	0	0
1	Л	500	Total	С	Ν	0	S	0	0	0
	D	099	4888	3186	822	866	14	0	0	0
1	F	604	Total	С	Ν	0	S	0	0	0
1	Ľ	004	4917	3202	830	871	14	0	0	
1	Б	502	Total	С	Ν	0	S	0	0	0
	Г	090	4859	3166	818	861	14	0	0	0
1	C	606	Total	С	Ν	0	S	0	0	0
	G	000	4923	3213	826	869	15	0	0	0
1	ц	603	Total	С	Ν	0	S	0	0	0
	п	005	4800	3138	791	857	14	0	0	

• Molecule 1 is a protein called 1,4-alpha-glucan branching enzyme GlgB.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0
2	В	34	Total O 34 34	0	0
2	С	31	$\begin{array}{cc} \text{Total} & \text{O} \\ 31 & 31 \end{array}$	0	0
2	D	27	TotalO2727	0	0
2	Ε	26	TotalO2626	0	0
2	F	51	$\begin{array}{cc} \text{Total} & \text{O} \\ 51 & 51 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
2	Н	24	Total O 24 24	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: 1,4-alpha-glucan branching enzyme GlgB













# R313 ASP SER SER SER CLYS GLU PRO ASN THR PRO ASN TLE GLY GLY L604 E605 L606 • Molecule 1: 1,4-alpha-glucan branching enzyme GlgB 2% Chain E: 73% 24% . . MET ARG MET ARG HIS TYR SER ARG LYS GLU TRP THR PRO ASN ILE PHC E475 W476 L545 F546 V547 L548 N477 H478



#### 

#### E518 E519 E519 E521 E521 E521 E521 E524 E533 E535 E546 E546 E546 E556 E556 E556 E556 E556 E556 E556 E568 E5688 E568 E5688 E568 E568 E568 E568 E568 E568 E568 E568











# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	100.30Å $112.27$ Å $166.26$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$73.59^{\circ}$ $73.77^{\circ}$ $65.25^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}\left(\mathring{\mathbf{A}}\right)$	100.10 - 2.91	Depositor
Resolution (A)	100.10 - 2.91	EDS
% Data completeness	98.9 (100.10-2.91)	Depositor
(in resolution range)	98.9(100.10-2.91)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.60 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
P. P.	0.197 , $0.256$	Depositor
$n, n_{free}$	0.208 , $0.250$	DCC
$R_{free}$ test set	129530 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	42.6	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , $61.2$	EDS
L-test for $twinning^2$	$<  L  > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.012 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	39395	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.22% 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		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.37	0/5080	0.63	0/6952	
1	В	0.35	0/5123	0.60	0/7011	
1	С	0.37	0/5121	0.62	0/7009	
1	D	0.38	0/5082	0.62	0/6952	
1	Ε	0.34	0/5112	0.61	0/6993	
1	F	0.35	0/5049	0.58	0/6902	
1	G	0.38	0/5118	0.64	0/7000	
1	Н	0.43	0/4993	0.67	0/6851	
All	All	0.37	0/40678	0.62	0/55670	

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	4886	0	4484	119	0
1	В	4925	0	4535	110	0
1	С	4925	0	4517	120	0
1	D	4888	0	4499	112	0
1	Е	4917	0	4523	110	0
1	F	4859	0	4500	127	0
1	G	4923	0	4527	113	0
1	Н	4800	0	4320	156	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	45	0	0	3	0
2	В	34	0	0	2	0
2	С	31	0	0	0	0
2	D	27	0	0	0	0
2	Е	26	0	0	1	0
2	F	51	0	0	1	0
2	G	34	0	0	1	0
2	Н	24	0	0	1	0
All	All	39395	0	35905	956	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 13.

All (956) 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:5:THR:HG22	1:D:7:GLU:H	1.16	1.05
1:F:15:GLY:HA2	1:F:284:ASN:HD21	1.33	0.94
1:H:154:TRP:HD1	1:H:466:MET:HE2	1.34	0.92
1:H:145:SER:H	1:H:182:THR:HG22	1.38	0.87
1:C:426:VAL:HG13	1:C:432:SER:HA	1.57	0.87
1:H:120:ARG:HB2	1:H:120:ARG:HH11	1.38	0.87
1:E:29:ASP:OD1	1:E:30:GLU:N	2.07	0.87
1:E:110:PRO:HG3	1:E:210:PHE:HZ	1.41	0.86
1:B:124:THR:HG21	1:E:541:ASP:HB2	1.57	0.84
1:D:5:THR:HG22	1:D:7:GLU:N	1.93	0.84
1:F:258:GLU:N	1:F:258:GLU:OE1	2.11	0.82
1:H:574:SER:HB3	1:H:613:ILE:H	1.43	0.82
1:E:357:GLU:OE2	1:E:359:THR:HB	1.80	0.81
1:D:83:LYS:HD2	1:D:94:ASP:HB3	1.62	0.81
1:H:456:TRP:HA	1:H:462:LYS:HE3	1.61	0.81
1:G:523:ILE:HD11	1:G:536:LEU:HG	1.64	0.80
1:H:562:VAL:HG23	1:H:602:PHE:HB2	1.65	0.79
1:D:145:SER:H	1:D:182:THR:HB	1.48	0.78
1:E:47:VAL:HG23	1:E:61:LEU:HD21	1.64	0.78
1:H:144:VAL:HG23	1:H:461:LYS:HB3	1.63	0.78
1:F:551:THR:HG22	1:F:553:VAL:H	1.48	0.78
1:B:554:PRO:HG3	1:B:610:PRO:HG3	1.65	0.77
1:C:456:TRP:HA	1:C:462:LYS:HE3	1.66	0.77
1:B:541:ASP:HB2	1:E:124:THR:HG21	1.65	0.77
1:B:357:GLU:OE2	1:B:359:THR:HB	1.83	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:144:VAL:HA	1:H:182:THR:HG21	1.65	0.76
1:D:155:ARG:HA	1:D:481:GLN:HG3	1.66	0.76
1:H:154:TRP:CD1	1:H:466:MET:HE2	2.20	0.76
1:D:182:THR:HG22	1:D:183:HIS:ND1	1.99	0.76
1:A:523:ILE:HD11	1:A:536:LEU:HD22	1.67	0.75
1:E:470:PHE:HZ	1:E:484:TRP:CZ3	2.06	0.74
1:F:19:ASP:OD2	1:F:22:ARG:NH2	2.20	0.74
1:G:17:PHE:HE1	1:G:19:ASP:HB2	1.52	0.74
1:E:466:MET:HB3	1:E:482:LEU:HD11	1.70	0.73
1:F:149:VAL:HA	1:F:466:MET:HE3	1.70	0.73
1:F:155:ARG:HA	1:F:481:GLN:HG3	1.71	0.73
1:H:144:VAL:CG2	1:H:461:LYS:HB3	2.17	0.73
1:E:28:PRO:HG3	1:E:118:ILE:HG22	1.71	0.73
1:G:540:THR:HG22	1:G:541:ASP:H	1.54	0.73
1:H:466:MET:HB2	1:H:482:LEU:HD11	1.70	0.73
1:D:352:ILE:HG23	1:D:376:LEU:HD23	1.72	0.72
1:H:9:ILE:HG21	1:H:65:GLY:HA3	1.70	0.71
1:H:559:ARG:HG2	1:H:603:HIS:CD2	2.25	0.71
1:B:466:MET:HB2	1:B:482:LEU:HD11	1.71	0.71
1:E:5:THR:HG22	1:E:7:GLU:H	1.56	0.71
1:H:521:GLU:HG2	1:H:600:ARG:HH22	1.56	0.71
1:A:126:HIS:HB2	1:A:227:GLN:OE1	1.91	0.71
1:E:533:ILE:HG23	1:E:548:LEU:HB2	1.73	0.70
1:B:19:ASP:OD2	1:B:22:ARG:NH2	2.21	0.70
1:B:338:LYS:HG2	1:B:368:THR:HG22	1.74	0.69
1:C:131:MET:HA	1:C:134:ARG:HG3	1.73	0.69
1:D:470:PHE:HZ	1:D:484:TRP:CZ3	2.09	0.69
1:B:570:GLU:OE2	1:B:614:LEU:HD23	1.92	0.69
1:F:303:ARG:HG2	1:F:354:ILE:HB	1.72	0.69
1:A:357:GLU:OE2	1:A:359:THR:HB	1.92	0.69
1:D:131:MET:HA	1:D:134:ARG:HG3	1.74	0.69
1:H:437:MET:HG3	1:H:447:ASN:HB3	1.75	0.69
1:D:87:ARG:NH1	1:D:89:GLY:O	2.25	0.69
1:B:574:SER:HB3	1:B:613:ILE:HG22	1.75	0.68
1:E:97:ASP:HB3	1:E:100:ALA:HB2	1.74	0.68
1:G:357:GLU:OE2	1:G:359:THR:HB	1.93	0.68
1:E:189:ILE:HD11	1:E:234:LEU:HD13	1.76	0.68
1:G:62:GLU:HG3	1:G:64:TYR:HE1	1.59	0.68
1:F:5:THR:HG22	1:F:8:ASP:H	1.59	0.68
1:G:5:THR:HG22	1:G:7:GLU:H	1.59	0.67
1:G:442:TRP:HE3	1:G:443:GLN:HG3	1.59	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:H:145:SER:H	1:H:182:THR:CG2	2.06	0.67
1:D:395:PRO:HA	1:D:398:ARG:HD2	1.76	0.67
1:E:131:MET:HA	1:E:134:ARG:HG3	1.77	0.67
1:H:357:GLU:OE2	1:H:359:THR:HB	1.95	0.67
1:C:234:LEU:HD22	1:C:299:VAL:HG11	1.76	0.67
1:H:33:THR:HG21	1:H:118:ILE:HG21	1.77	0.67
1:H:193:PRO:HD3	1:H:203:VAL:HG13	1.75	0.67
1:A:307:VAL:HG21	1:A:355:ALA:HB1	1.77	0.67
1:B:548:LEU:HG	1:B:613:ILE:HG13	1.76	0.67
1:E:383:TRP:CH2	1:E:455:MET:HG3	2.29	0.67
1:G:378:LYS:HD3	1:G:417:TYR:HE1	1.60	0.67
1:H:255:THR:HA	1:H:258:GLU:OE1	1.94	0.66
1:B:165:TYR:HB2	1:B:217:ASP:HB3	1.75	0.66
1:H:144:VAL:HG22	1:H:461:LYS:HD2	1.77	0.66
1:C:554:PRO:HD3	1:C:610:PRO:HG3	1.76	0.66
1:G:448:LEU:HD23	1:G:495:ILE:HD13	1.76	0.66
1:E:183:HIS:CD2	1:E:231:GLY:HA3	2.30	0.66
1:F:198:TRP:HH2	1:F:427:VAL:HG21	1.60	0.66
1:F:17:PHE:N	1:F:284:ASN:OD1	2.28	0.66
1:D:189:ILE:HD11	1:D:234:LEU:HD13	1.78	0.66
1:E:139:SER:HA	1:E:142:GLU:HG3	1.77	0.66
1:F:165:TYR:HB2	1:F:217:ASP:HB3	1.77	0.66
1:H:391:MET:HE1	1:H:451:LEU:HB2	1.78	0.65
1:E:145:SER:H	1:E:182:THR:HB	1.60	0.65
1:F:63:ARG:NH1	1:F:64:TYR:O	2.29	0.65
1:F:518:GLU:HG3	1:F:519:GLY:H	1.60	0.65
1:H:437:MET:HG3	1:H:447:ASN:CB	2.26	0.65
1:E:11:ARG:NH2	1:E:19:ASP:OD1	2.29	0.65
1:F:241:PHE:HB3	1:F:275:PHE:CZ	2.32	0.65
1:H:469:GLU:OE1	1:H:469:GLU:N	2.22	0.65
1:B:142:GLU:OE2	1:E:133:ARG:HD3	1.96	0.65
1:D:24:LEU:HA	1:D:36:CYS:HB3	1.78	0.65
1:E:182:THR:HG22	1:E:183:HIS:ND1	2.11	0.65
1:G:313:ARG:HG3	1:G:328:ARG:O	1.97	0.65
1:C:352:ILE:HG23	1:C:376:LEU:HD23	1.78	0.65
1:C:562:VAL:HG23	1:C:602:PHE:HB2	1.79	0.65
1:D:28:PRO:HG3	1:D:118:ILE:HG22	1.79	0.65
1:F:405:LEU:HD21	1:F:533:ILE:HG13	1.79	0.64
1:C:545:LEU:HD23	1:C:616:LEU:HD13	1.79	0.64
1:D:442:TRP:HD1	1:D:491:TYR:HH	1.45	0.64
1:F:474:HIS:ND1	1:F:483:GLU:OE2	2.29	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:154:TRP:HD1	1:C:466:MET:HE2	1.63	0.64
1:G:554:PRO:HG3	1:G:610:PRO:HG3	1.80	0.64
1:H:9:ILE:HD13	1:H:65:GLY:H	1.63	0.64
1:H:568:TRP:CD1	1:H:604:LEU:HD21	2.33	0.64
1:H:408:SER:OG	1:H:458:HIS:NE2	2.30	0.63
1:E:303:ARG:HG2	1:E:354:ILE:HB	1.81	0.63
1:G:587:PHE:HA	2:G:718:HOH:O	1.99	0.63
1:H:165:TYR:HB2	1:H:217:ASP:HB3	1.80	0.63
1:A:19:ASP:HB3	1:A:22:ARG:HD3	1.79	0.63
1:F:254:THR:HG22	1:F:255:THR:H	1.64	0.63
1:E:574:SER:HB3	1:E:613:ILE:H	1.63	0.63
1:H:505:LEU:HD11	1:H:544:LEU:HD21	1.81	0.63
1:H:153:SER:OG	1:H:478:HIS:HA	1.98	0.63
1:F:395:PRO:HA	1:F:398:ARG:HD2	1.79	0.62
1:A:155:ARG:HA	1:A:481:GLN:HG3	1.81	0.62
1:G:24:LEU:HA	1:G:36:CYS:HB3	1.81	0.62
1:H:120:ARG:HB2	1:H:120:ARG:NH1	2.13	0.62
1:H:434:TRP:HA	1:H:448:LEU:HD11	1.81	0.62
1:A:519:GLY:O	1:A:537:ARG:HA	1.99	0.62
1:B:437:MET:HE3	1:B:447:ASN:HB3	1.82	0.62
1:A:5:THR:O	1:A:9:ILE:HD12	1.98	0.62
1:C:177:GLN:OE1	1:C:228:ARG:NH2	2.29	0.62
1:G:334:ILE:HG22	1:G:338:LYS:HD2	1.81	0.62
1:C:183:HIS:CD2	1:C:231:GLY:HA3	2.35	0.62
1:H:154:TRP:CH2	1:H:172:LEU:HA	2.34	0.62
1:C:250:TYR:HA	1:C:254:THR:O	1.99	0.62
1:A:554:PRO:HB3	1:A:584:MET:HE1	1.80	0.62
1:C:574:SER:HB3	1:C:613:ILE:CG2	2.30	0.61
1:D:153:SER:HB2	1:D:466:MET:HE1	1.81	0.61
1:G:559:ARG:HB3	1:G:603:HIS:CD2	2.35	0.61
1:C:575:ASP:OD2	1:C:609:PRO:HB3	2.01	0.61
1:B:504:HIS:O	1:B:508:THR:HG23	2.00	0.61
1:D:522:TRP:HZ3	1:D:533:ILE:HG23	1.65	0.61
1:D:303:ARG:HG2	1:D:354:ILE:HB	1.82	0.61
1:H:291:LEU:HD21	1:H:343:THR:HG22	1.83	0.61
1:G:153:SER:O	1:G:481:GLN:HA	2.01	0.61
1:D:256:LEU:O	1:D:279:LYS:NZ	2.32	0.60
1:G:313:ARG:HG2	1:G:330:ASN:HB2	1.83	0.60
1:A:3:TRP:H	1:A:64:TYR:HE2	1.48	0.60
1:C:551:THR:CG2	$1:\overline{C:553:VAL:HG22}$	2.32	0.60
1:G:440:ASP:O	1:G:444:LYS:HG3	2.01	0.60



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:95:LYS:NZ	1:C:245:PRO:O	2.34	0.60
1:F:257:PHE:N	1:F:258:GLU:OE1	2.35	0.60
1:H:304:VAL:HG12	1:H:307:VAL:HG22	1.83	0.60
1:H:97:ASP:HB3	1:H:100:ALA:HB2	1.83	0.60
1:A:378:LYS:HD3	1:A:415:GLU:HG3	1.84	0.59
1:A:48:LEU:HD11	1:A:56:PRO:HA	1.85	0.59
1:A:303:ARG:HG3	1:A:354:ILE:HB	1.84	0.59
1:F:15:GLY:CA	1:F:284:ASN:HD21	2.13	0.59
1:E:470:PHE:CZ	1:E:484:TRP:CZ3	2.90	0.59
1:F:48:LEU:HD21	1:F:56:PRO:HA	1.83	0.59
1:F:178:ASP:CG	1:F:500:ARG:HH21	2.06	0.59
1:C:527:ASP:OD1	1:C:530:GLN:HB2	2.02	0.59
1:E:443:GLN:O	1:E:447:ASN:ND2	2.35	0.59
1:G:255:THR:HG22	1:G:258:GLU:HB2	1.85	0.59
1:F:148:GLU:HB3	1:F:465:PHE:HA	1.85	0.59
1:B:524:ASP:HB2	1:B:598:HIS:CD2	2.38	0.58
1:H:15:GLY:HA2	1:H:284:ASN:OD1	2.03	0.58
1:F:521:GLU:OE1	1:F:600:ARG:NH2	2.32	0.58
1:B:523:ILE:HD11	1:B:536:LEU:HD13	1.86	0.58
1:G:389:ASP:OD2	1:G:393:ARG:NH2	2.37	0.58
1:H:398:ARG:NH1	1:H:550:PHE:O	2.36	0.58
1:H:545:LEU:HD23	1:H:616:LEU:HD23	1.83	0.58
1:D:109:SER:HB3	1:D:112:GLU:HG3	1.85	0.58
1:A:96:THR:HG22	1:C:91:TYR:OH	2.03	0.58
1:B:609:PRO:HD2	1:B:614:LEU:HD11	1.85	0.58
1:C:346:LEU:HD23	1:C:347:HIS:CE1	2.38	0.58
1:D:131:MET:HG2	1:D:134:ARG:HD3	1.86	0.58
1:F:208:PRO:HB3	1:F:218:LEU:HD22	1.85	0.58
1:G:512:LEU:HD23	1:G:537:ARG:HG2	1.84	0.58
1:H:182:THR:HG23	1:H:183:HIS:ND1	2.19	0.58
1:F:192:HIS:O	1:F:211:ARG:NH2	2.36	0.58
1:D:6:GLU:CD	1:D:6:GLU:H	2.05	0.58
1:G:29:ASP:OD1	1:G:72:TYR:HE1	1.87	0.58
1:G:388:LEU:O	1:G:392:ARG:HG3	2.04	0.58
1:A:521:GLU:OE2	1:A:600:ARG:NH1	2.36	0.58
1:D:48:LEU:HD21	1:D:56:PRO:HA	1.85	0.58
1:H:466:MET:HB2	1:H:482:LEU:CD1	2.33	0.58
1:G:192:HIS:CE1	1:G:211:ARG:HH22	2.22	0.58
1:A:24:LEU:HA	1:A:36:CYS:HB3	1.86	0.57
1:B:47:VAL:HG23	1:B:61:LEU:HD21	1.86	0.57
1:B:48:LEU:HB2	1:B:83:LYS:HG3	1.86	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:177:GLN:HE22	1:A:228:ARG:HE	1.51	0.57
1:C:104:GLU:HG3	1:C:117:ILE:HD13	1.86	0.57
1:F:564:ILE:HG22	1:F:568:TRP:CZ2	2.39	0.57
1:A:177:GLN:NE2	1:A:228:ARG:HE	2.03	0.57
1:E:47:VAL:CG2	1:E:61:LEU:HD21	2.34	0.57
1:D:552:PRO:HG3	1:D:611:LEU:HD11	1.86	0.57
1:F:244:ASP:OD2	1:F:246:GLN:N	2.38	0.57
1:C:551:THR:HG21	1:C:553:VAL:HG22	1.87	0.57
1:E:522:TRP:CH2	1:E:533:ILE:HD11	2.39	0.57
1:F:41:HIS:ND1	1:F:252:ASP:OD2	2.38	0.57
1:C:6:GLU:CD	1:C:6:GLU:H	2.08	0.57
1:A:85:ARG:HD3	1:A:94:ASP:OD1	2.05	0.57
1:D:63:ARG:HD2	1:D:69:TRP:CZ2	2.40	0.57
1:E:110:PRO:HG3	1:E:210:PHE:CZ	2.32	0.57
1:F:48:LEU:HB2	1:F:83:LYS:HG2	1.86	0.57
1:G:440:ASP:OD2	1:G:443:GLN:NE2	2.38	0.57
1:G:442:TRP:HH2	1:G:610:PRO:HB2	1.70	0.57
1:H:241:PHE:HZ	1:H:258:GLU:HG3	1.70	0.57
1:B:244:ASP:HB3	1:B:246:GLN:HE22	1.70	0.56
1:C:486:LEU:HB3	1:C:492:HIS:ND1	2.20	0.56
1:D:551:THR:HG21	1:D:555:ARG:HH21	1.70	0.56
1:D:555:ARG:HB2	1:D:608:LEU:HB2	1.85	0.56
1:C:149:VAL:HA	1:C:466:MET:HE3	1.87	0.56
1:C:308:ALA:HB2	1:C:357:GLU:OE2	2.04	0.56
1:C:339:LYS:O	1:C:343:THR:HG23	2.05	0.56
1:G:3:TRP:HB2	1:G:34:TRP:CZ3	2.40	0.56
1:G:95:LYS:NZ	1:G:249:VAL:O	2.33	0.56
1:H:28:PRO:HG3	1:H:118:ILE:HG22	1.87	0.56
1:C:460:GLY:O	1:C:462:LYS:NZ	2.26	0.56
1:B:559:ARG:HB3	1:B:603:HIS:CD2	2.40	0.56
1:C:154:TRP:CD1	1:C:466:MET:HE2	2.40	0.56
1:E:546:PHE:HD2	1:E:613:ILE:HD11	1.70	0.56
1:G:241:PHE:HZ	1:G:258:GLU:HG3	1.70	0.56
1:A:584:MET:HE2	1:A:610:PRO:HD3	1.86	0.56
1:B:267:HIS:HE1	1:B:269:ASP:HB2	1.71	0.56
1:B:440:ASP:O	1:B:444:LYS:HG3	2.06	0.56
1:E:267:HIS:CE1	1:E:309:SER:HB2	2.41	0.56
1:F:518:GLU:HG3	1:F:519:GLY:N	2.20	0.56
1:G:437:MET:O	1:G:444:LYS:HE3	2.05	0.56
1:H:307:VAL:HG21	1:H:355:ALA:HB1	1.88	0.56
1:F:49:GLY:HA3	1:F:51:PHE:CE1	2.41	0.56



	is as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:388:LEU:O	1:F:392:ARG:HG3	2.05	0.56
1:G:102:ALA:HB3	1:G:119:THR:HG21	1.88	0.56
1:A:52:ASN:HD22	1:A:59:HIS:HD2	1.54	0.56
1:B:597:TRP:HD1	1:B:598:HIS:ND1	2.04	0.56
1:B:154:TRP:HD1	1:B:466:MET:HE2	1.71	0.56
1:F:577:VAL:HG22	2:F:709:HOH:O	2.05	0.55
1:A:241:PHE:HZ	1:A:258:GLU:HG3	1.72	0.55
1:F:419:LEU:N	1:F:461:LYS:O	2.36	0.55
1:A:157:LYS:HG2	1:A:163:PHE:CE1	2.41	0.55
1:F:5:THR:HG22	1:F:8:ASP:N	2.21	0.55
1:H:192:HIS:CD2	1:H:199:GLY:HA2	2.41	0.55
1:B:576:ALA:HB3	1:B:579:TYR:CD2	2.42	0.55
1:E:333:ALA:O	1:E:337:ILE:HG13	2.06	0.55
1:H:214:THR:HG22	1:H:215:PRO:HD2	1.89	0.55
1:C:155:ARG:HG2	1:C:484:TRP:NE1	2.22	0.55
1:G:594:PRO:HA	1:G:602:PHE:CD1	2.41	0.55
1:F:5:THR:HG23	1:F:7:GLU:H	1.71	0.55
1:C:51:PHE:CD1	1:C:73:VAL:HG11	2.42	0.55
1:F:147:TYR:OH	1:F:469:GLU:OE2	2.21	0.55
1:C:37:VAL:HG11	1:C:45:VAL:HG11	1.89	0.55
1:C:574:SER:HB3	1:C:613:ILE:HG22	1.89	0.55
1:E:232:VAL:N	1:E:300:ASP:OD2	2.30	0.55
1:D:470:PHE:CZ	1:D:484:TRP:CZ3	2.94	0.55
1:E:7:GLU:O	1:E:11:ARG:HG3	2.06	0.55
1:H:120:ARG:HH11	1:H:120:ARG:CB	2.14	0.55
1:H:293:TRP:O	1:H:299:VAL:HG22	2.06	0.55
1:H:394:ASP:O	1:H:398:ARG:HG3	2.07	0.55
1:F:63:ARG:HG3	1:F:69:TRP:CE2	2.42	0.54
1:F:548:LEU:HG	1:F:613:ILE:HB	1.89	0.54
1:H:571:VAL:CG2	1:H:617:GLU:HB3	2.38	0.54
1:F:154:TRP:HD1	1:F:466:MET:HE2	1.73	0.54
1:F:198:TRP:CH2	1:F:427:VAL:HG21	2.42	0.54
1:B:267:HIS:CE1	1:B:269:ASP:HB2	2.41	0.54
1:H:571:VAL:HG21	1:H:617:GLU:HB3	1.89	0.54
1:H:17:PHE:H	1:H:284:ASN:HD21	1.55	0.54
1:H:105:PRO:HA	1:H:114:LEU:HA	1.89	0.54
1:C:174:ASP:OD1	1:C:228:ARG:NH2	2.34	0.54
1:E:522:TRP:CZ3	1:E:533:ILE:CD1	2.91	0.54
1:F:250:TYR:HA	1:F:258:GLU:OE2	2.06	0.54
1:H:426:VAL:HG13	1:H:432:SER:HA	1.89	0.54
1:A:174:ASP:OD1	1:A:228:ARG:NH2	2.40	0.54



	hi a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:395:PRO:HA	1:G:398:ARG:HD2	1.90	0.54
1:A:313:ARG:HG2	1:A:330:ASN:HB2	1.90	0.54
1:E:153:SER:HB2	1:E:466:MET:HE1	1.90	0.54
1:A:214:THR:HG23	1:A:215:PRO:HD2	1.90	0.53
1:A:330:ASN:O	1:A:334:ILE:HG13	2.08	0.53
1:C:582:SER:HB3	1:C:584:MET:HG3	1.89	0.53
1:G:383:TRP:O	1:G:387:THR:OG1	2.21	0.53
1:C:3:TRP:HB2	1:C:34:TRP:CZ3	2.43	0.53
1:D:11:ARG:NH2	1:D:19:ASP:OD1	2.41	0.53
1:F:63:ARG:HG3	1:F:69:TRP:CZ2	2.43	0.53
1:F:250:TYR:N	1:F:258:GLU:OE2	2.41	0.53
1:F:258:GLU:H	1:F:258:GLU:CD	2.10	0.53
1:A:150:HIS:HA	2:A:708:HOH:O	2.08	0.53
1:D:20:SER:HB2	1:D:24:LEU:HD12	1.91	0.53
1:E:491:TYR:O	1:E:495:ILE:HD12	2.09	0.53
1:G:466:MET:HB3	1:G:482:LEU:HD11	1.90	0.53
1:C:575:ASP:OD1	1:C:582:SER:N	2.37	0.53
1:H:524:ASP:OD2	1:H:598:HIS:CD2	2.62	0.53
1:B:192:HIS:CG	1:B:199:GLY:HA2	2.44	0.53
1:D:95:LYS:NZ	1:D:249:VAL:O	2.35	0.53
1:F:218:LEU:HD23	1:F:297:TYR:CE2	2.44	0.53
1:H:565:GLY:HA2	1:H:592:ALA:HB3	1.90	0.53
1:F:175:TYR:O	1:F:179:LEU:HD12	2.09	0.53
1:B:107:THR:HG22	1:D:490:PRO:HB3	1.90	0.53
1:G:307:VAL:HG21	1:G:355:ALA:HB1	1.91	0.53
1:G:518:GLU:CD	1:G:518:GLU:H	2.11	0.53
1:H:3:TRP:HB2	1:H:34:TRP:CZ3	2.44	0.53
1:A:97:ASP:HB3	1:A:100:ALA:HB2	1.91	0.53
1:F:564:ILE:HG22	1:F:568:TRP:HZ2	1.73	0.53
1:G:134:ARG:HH11	1:G:300:ASP:HA	1.72	0.53
1:A:574:SER:HB3	1:A:613:ILE:H	1.74	0.53
1:D:77:LEU:HB2	1:D:80:HIS:ND1	2.24	0.53
1:G:540:THR:HG22	1:G:541:ASP:N	2.21	0.53
1:E:152:GLY:HA3	1:E:195:TYR:OH	2.09	0.53
1:E:255:THR:HA	1:E:258:GLU:OE2	2.09	0.53
1:F:154:TRP:CD1	1:F:466:MET:HE2	2.43	0.53
1:H:149:VAL:HG13	1:H:466:MET:HE1	1.90	0.53
1:C:250:TYR:HE1	1:C:255:THR:HG22	1.72	0.52
1:H:390:TYR:HE2	1:H:550:PHE:CD2	2.27	0.52
1:B:436:LYS:NZ	2:B:701:HOH:O	2.27	0.52
1:C:473:HIS:NE2	1:C:492:HIS:HE1	2.07	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:244:ASP:HB3	1:A:247:GLY:H	1.73	0.52
1:D:570:GLU:HB2	1:D:588:GLY:H	1.73	0.52
1:H:169:ALA:HB1	1:H:224:TYR:HD2	1.74	0.52
1:A:214:THR:HG22	1:A:216:GLN:H	1.73	0.52
1:E:196:GLY:HA2	1:E:478:HIS:NE2	2.25	0.52
1:F:105:PRO:HA	1:F:114:LEU:H	1.74	0.52
1:B:395:PRO:HA	1:B:398:ARG:HG3	1.92	0.52
1:H:419:LEU:N	1:H:461:LYS:O	2.41	0.52
1:D:395:PRO:HB3	1:D:551:THR:HA	1.90	0.52
1:E:304:VAL:HG12	1:E:307:VAL:HG22	1.91	0.52
1:H:426:VAL:HG12	1:H:426:VAL:O	2.10	0.52
1:A:253:GLY:O	1:C:245:PRO:HG3	2.10	0.52
1:C:15:GLY:HA2	1:C:284:ASN:ND2	2.24	0.52
1:E:176:VAL:HG13	1:E:181:PHE:HB2	1.91	0.52
1:F:250:TYR:HA	1:F:254:THR:O	2.10	0.52
1:H:192:HIS:CG	1:H:199:GLY:HA2	2.45	0.52
1:H:573:ASN:HD21	1:H:585:GLY:HA2	1.75	0.52
1:C:103:MET:HB2	1:C:191:GLU:HG2	1.92	0.52
1:E:49:GLY:HA2	1:E:54:TRP:CZ3	2.45	0.52
1:E:95:LYS:NZ	1:E:245:PRO:O	2.43	0.52
1:G:456:TRP:HA	1:G:462:LYS:HD2	1.92	0.52
1:E:334:ILE:O	1:E:338:LYS:HG3	2.09	0.52
1:G:521:GLU:OE2	1:G:600:ARG:NH1	2.38	0.51
1:A:9:ILE:HG12	1:A:65:GLY:HA3	1.90	0.51
1:B:267:HIS:HB3	1:B:271:GLY:HA2	1.92	0.51
1:B:456:TRP:HA	1:B:462:LYS:CE	2.39	0.51
1:B:95:LYS:NZ	1:B:249:VAL:O	2.43	0.51
1:B:480:THR:HG22	1:B:481:GLN:H	1.75	0.51
1:E:307:VAL:HG21	1:E:355:ALA:HB1	1.92	0.51
1:G:18:TYR:HB3	1:G:291:LEU:HD12	1.92	0.51
1:A:7:GLU:O	1:A:11:ARG:HG3	2.09	0.51
1:A:178:ASP:O	1:A:500:ARG:HG3	2.11	0.51
1:A:554:PRO:CB	1:A:584:MET:HE1	2.39	0.51
1:C:405:LEU:HD21	1:C:533:ILE:HD13	1.93	0.51
1:F:402:HIS:O	1:F:406:THR:HG23	2.10	0.51
1:D:278:ASN:ND2	1:D:332:GLU:HG2	2.25	0.51
1:H:498:TRP:CZ3	1:H:572:LEU:HD13	2.46	0.51
1:B:179:LEU:HD21	1:B:496:GLN:HG3	1.92	0.51
1:E:432:SER:OG	1:E:472:GLN:O	2.23	0.51
1:H:33:THR:HG23	1:H:76:ALA:O	2.10	0.51
1:A:197:SER:HB2	1:A:201:GLN:HG2	1.93	0.51



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:151:LEU:HD22	1:D:168:ILE:HD13	1.92	0.51
1:D:189:ILE:HD11	1:D:234:LEU:CD1	2.41	0.51
1:F:546:PHE:HD2	1:F:613:ILE:HD11	1.76	0.51
1:G:153:SER:CB	1:G:476:TRP:HE1	2.24	0.51
1:F:12:TRP:HD1	1:F:66:ALA:HB1	1.76	0.50
1:F:551:THR:HG22	1:F:553:VAL:N	2.24	0.50
1:D:559:ARG:HA	1:D:604:LEU:O	2.11	0.50
1:G:216:GLN:CD	1:G:216:GLN:H	2.15	0.50
1:H:24:LEU:HA	1:H:36:CYS:HB3	1.93	0.50
1:A:4:LEU:HD12	1:A:64:TYR:HB2	1.94	0.50
1:B:534:CYS:HA	1:B:546:PHE:O	2.11	0.50
1:D:409:LEU:HD13	1:D:522:TRP:CZ2	2.45	0.50
1:F:352:ILE:HG23	1:F:376:LEU:HD23	1.92	0.50
1:A:192:HIS:CG	1:A:199:GLY:HA2	2.47	0.50
1:C:13:GLU:HG3	1:C:66:ALA:HB2	1.92	0.50
1:E:424:ASP:O	1:E:430:LYS:HE3	2.12	0.50
1:H:41:HIS:HB2	1:H:252:ASP:OD2	2.12	0.50
1:B:456:TRP:HA	1:B:462:LYS:HE2	1.94	0.50
1:C:134:ARG:HD2	1:C:300:ASP:OD1	2.12	0.50
1:D:18:TYR:HB3	1:D:291:LEU:HD12	1.94	0.50
1:F:106:PRO:HD2	1:F:113:GLY:HA3	1.92	0.50
1:G:248:LEU:HB3	1:G:257:PHE:CD2	2.47	0.50
1:A:104:GLU:HB2	1:A:117:ILE:HD11	1.93	0.50
1:B:267:HIS:HB3	1:B:271:GLY:N	2.27	0.50
1:C:12:TRP:HZ2	1:C:38:TRP:CD2	2.30	0.50
1:C:473:HIS:NE2	1:C:492:HIS:CE1	2.80	0.50
1:D:540:THR:OG1	1:D:541:ASP:N	2.44	0.50
1:E:250:TYR:HA	1:E:258:GLU:OE2	2.12	0.50
1:F:164:SER:HB3	1:F:167:GLU:HB2	1.93	0.50
1:H:167:GLU:O	1:H:171:PRO:HD2	2.11	0.50
1:A:311:LEU:HD13	1:A:361:TRP:CD2	2.46	0.50
1:H:189:ILE:HD12	1:H:190:MET:HG3	1.93	0.50
1:A:139:SER:HA	1:A:142:GLU:HG3	1.93	0.50
1:D:391:MET:HG3	1:D:451:LEU:HD12	1.94	0.50
1:E:120:ARG:HH11	1:E:120:ARG:HG3	1.77	0.50
1:E:136:GLY:HA2	1:E:352:ILE:HD11	1.92	0.50
1:B:47:VAL:CG2	1:B:61:LEU:HD21	2.42	0.49
1:D:77:LEU:HB2	1:D:80:HIS:CE1	2.47	0.49
1:H:37:VAL:HG11	1:H:45:VAL:HG11	1.94	0.49
1:H:521:GLU:HB3	1:H:536:LEU:HB3	1.94	0.49
1:C:61:LEU:HD22	1:C:71:GLY:HA3	1.93	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:95:LYS:HD2	1:A:246:GLN:O	2.13	0.49
1:B:395:PRO:HB3	1:B:551:THR:HA	1.94	0.49
1:D:3:TRP:HB2	1:D:34:TRP:CZ3	2.48	0.49
1:D:480:THR:OG1	1:D:481:GLN:N	2.45	0.49
1:G:427:VAL:HG11	1:G:476:TRP:HE3	1.77	0.49
1:E:135:LYS:HA	1:E:135:LYS:HE2	1.94	0.49
1:B:267:HIS:HB3	1:B:271:GLY:CA	2.43	0.49
1:C:5:THR:HG22	1:C:7:GLU:H	1.76	0.49
1:C:465:PHE:CE1	1:C:466:MET:HG2	2.47	0.49
1:F:202:VAL:N	1:F:242:ALA:HB2	2.28	0.49
1:F:284:ASN:H	1:F:284:ASN:HD22	1.59	0.49
1:H:169:ALA:HB2	1:H:221:LEU:HD12	1.94	0.49
1:A:574:SER:HB2	1:A:613:ILE:HG23	1.94	0.49
1:B:154:TRP:CD1	1:B:466:MET:HE2	2.47	0.49
1:D:214:THR:HG22	1:D:217:ASP:H	1.77	0.49
1:D:215:PRO:O	1:D:219:MET:HG3	2.12	0.49
1:E:175:TYR:OH	1:E:470:PHE:HE1	1.95	0.49
1:G:459:PRO:HA	1:G:537:ARG:NH2	2.28	0.49
1:B:103:MET:HB2	1:B:191:GLU:HG2	1.94	0.49
1:C:143:PRO:HD3	1:C:513:TRP:CE2	2.46	0.49
1:E:469:GLU:O	1:E:495:ILE:HG22	2.13	0.49
1:G:594:PRO:HA	1:G:602:PHE:HD1	1.77	0.49
1:A:527:ASP:OD1	1:A:530:GLN:HG3	2.12	0.49
1:B:153:SER:O	1:B:481:GLN:HA	2.12	0.49
1:C:395:PRO:HA	1:C:398:ARG:HD2	1.93	0.49
1:H:391:MET:CE	1:H:451:LEU:HB2	2.41	0.49
1:B:19:ASP:OD2	1:B:22:ARG:NE	2.45	0.49
1:B:140:LEU:HD21	1:B:416:HIS:CG	2.48	0.49
1:E:278:ASN:OD1	1:E:332:GLU:HG2	2.13	0.49
1:G:143:PRO:HD3	1:G:513:TRP:CE2	2.47	0.49
1:H:291:LEU:O	1:H:295:ASP:N	2.43	0.49
1:H:294:LEU:HD23	1:H:299:VAL:HG23	1.95	0.49
1:A:37:VAL:HG22	1:A:84:TYR:CZ	2.48	0.49
1:B:355:ALA:HB2	1:B:375:PHE:CD2	2.48	0.49
1:D:130:TRP:HD1	1:D:131:MET:HG3	1.78	0.49
1:E:49:GLY:HA3	1:E:51:PHE:CE1	2.48	0.49
1:E:395:PRO:HA	1:E:398:ARG:HD2	1.95	0.49
1:G:150:HIS:ND1	1:G:153:SER:OG	2.34	0.49
1:G:378:LYS:HD3	1:G:417:TYR:CE1	2.44	0.49
1:B:148:GLU:HB2	1:B:463:LEU:HD21	1.95	0.48
1:C:307:VAL:HG21	1:C:355:ALA:HB1	1.95	0.48



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:399:LYS:HD2	1:F:400:TYR:CZ	2.47	0.48
1:F:406:THR:HG22	1:F:533:ILE:HD11	1.94	0.48
1:G:187:LEU:HD23	1:G:200:TYR:HE2	1.78	0.48
1:E:245:PRO:HG2	1:E:246:GLN:NE2	2.28	0.48
1:E:522:TRP:CH2	1:E:533:ILE:CD1	2.96	0.48
1:H:270:TRP:HD1	1:H:274:VAL:HG22	1.78	0.48
1:A:453:GLY:HA3	1:A:613:ILE:HG21	1.94	0.48
1:D:406:THR:HG22	1:D:533:ILE:HD11	1.95	0.48
1:E:201:GLN:C	1:E:242:ALA:HB2	2.34	0.48
1:E:544:LEU:HD22	1:E:615:ILE:HG22	1.94	0.48
1:H:61:LEU:HD22	1:H:71:GLY:HA3	1.95	0.48
1:H:365:SER:OG	1:H:415:GLU:HB3	2.13	0.48
1:B:165:TYR:CZ	1:B:212:TYR:HB2	2.49	0.48
1:B:403:ASP:CG	1:B:528:ARG:HH22	2.16	0.48
1:B:431:GLY:O	1:B:436:LYS:HE2	2.13	0.48
1:C:394:ASP:OD1	1:C:396:VAL:HG22	2.14	0.48
1:D:584:MET:HG3	1:D:610:PRO:HD3	1.95	0.48
1:G:596:SER:O	1:G:597:TRP:HE3	1.95	0.48
1:H:601:PRO:HB2	1:H:602:PHE:CD1	2.49	0.48
1:H:35:PHE:HZ	1:H:118:ILE:HD11	1.79	0.48
1:G:17:PHE:CE1	1:G:19:ASP:HB2	2.41	0.48
1:H:267:HIS:ND1	1:H:268:PRO:HD2	2.29	0.48
1:A:270:TRP:HD1	1:A:274:VAL:HG22	1.79	0.48
1:A:473:HIS:HB3	1:H:31:GLU:OE2	2.14	0.48
1:D:457:GLY:O	1:D:537:ARG:HD2	2.13	0.48
1:G:3:TRP:O	1:G:23:LYS:HE2	2.14	0.48
1:G:258:GLU:CD	1:G:258:GLU:H	2.16	0.48
1:H:125:TRP:CD2	1:H:298:HIS:CD2	3.01	0.48
1:A:151:LEU:HD22	1:A:168:ILE:HD13	1.94	0.48
1:A:163:PHE:HD1	1:A:167:GLU:HB3	1.79	0.48
1:A:424:ASP:HB2	2:A:715:HOH:O	2.13	0.48
1:A:506:TYR:HA	1:A:512:LEU:HD12	1.96	0.48
1:C:473:HIS:HB2	1:C:474:HIS:CD2	2.48	0.48
1:D:96:THR:HG22	1:D:246:GLN:O	2.14	0.48
1:B:59:HIS:CG	1:B:73:VAL:HG22	2.49	0.48
1:C:35:PHE:CE2	1:C:47:VAL:HG11	2.49	0.48
1:C:193:PRO:HG3	1:C:203:VAL:HG21	1.96	0.48
1:C:392:ARG:HG2	1:C:392:ARG:HH11	1.78	0.48
1:C:418:ILE:HG12	1:C:461:LYS:HB2	1.96	0.48
1:C:511:ALA:HB1	1:C:537:ARG:O	2.14	0.48
1:D:15:GLY:HA2	1:D:284:ASN:ND2	2.28	0.48



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:449:ARG:HG3	1:D:495:ILE:HG12	1.96	0.48
1:E:175:TYR:HH	1:E:470:PHE:HE1	1.58	0.48
1:F:90:PHE:HB3	1:F:91:TYR:CE2	2.49	0.48
1:A:111:ILE:HD12	1:A:111:ILE:H	1.79	0.47
1:E:99:TYR:CE1	1:E:285:PHE:HD1	2.32	0.47
1:F:249:VAL:HG12	1:F:250:TYR:CD2	2.49	0.47
1:H:472:GLN:HE22	1:H:482:LEU:HD22	1.78	0.47
1:C:56:PRO:HB3	1:C:85:ARG:HD2	1.94	0.47
1:E:245:PRO:HG2	1:E:246:GLN:HE21	1.78	0.47
1:F:7:GLU:O	1:F:11:ARG:HG3	2.15	0.47
1:A:3:TRP:O	1:A:23:LYS:NZ	2.40	0.47
1:A:568:TRP:HB2	1:A:590:VAL:HG13	1.94	0.47
1:B:62:GLU:HB3	1:B:64:TYR:HE2	1.78	0.47
1:C:7:GLU:O	1:C:11:ARG:HG3	2.14	0.47
1:G:442:TRP:CE3	1:G:443:GLN:HG3	2.44	0.47
1:A:157:LYS:HD3	1:A:167:GLU:OE1	2.14	0.47
1:A:562:VAL:HG11	1:A:604:LEU:HG	1.96	0.47
1:C:552:PRO:O	1:C:610:PRO:HB3	2.15	0.47
1:D:331:LEU:H	1:D:331:LEU:HD12	1.79	0.47
1:E:559:ARG:HA	1:E:604:LEU:O	2.15	0.47
1:H:574:SER:HB2	1:H:613:ILE:HG22	1.96	0.47
1:G:255:THR:HA	1:G:258:GLU:OE1	2.14	0.47
1:H:190:MET:HE3	1:H:190:MET:H	1.80	0.47
1:B:271:GLY:C	1:B:273:TYR:H	2.17	0.47
1:C:573:ASN:OD1	1:C:614:LEU:HD22	2.15	0.47
1:D:523:ILE:HD11	1:D:536:LEU:HD13	1.95	0.47
1:E:545:LEU:HD12	1:E:546:PHE:N	2.29	0.47
1:H:246:GLN:H	1:H:246:GLN:HG3	1.33	0.47
1:H:423:HIS:HB3	1:H:465:PHE:CE1	2.50	0.47
1:A:419:LEU:N	1:A:461:LYS:O	2.42	0.47
1:D:153:SER:CB	1:D:476:TRP:HE1	2.28	0.47
1:D:157:LYS:HG2	1:D:163:PHE:CE1	2.50	0.47
1:E:51:PHE:CD2	1:E:73:VAL:HG11	2.50	0.47
1:E:440:ASP:OD2	1:E:443:GLN:HG3	2.15	0.47
1:G:313:ARG:NH1	1:G:332:GLU:OE2	2.46	0.47
1:H:192:HIS:CD2	1:H:211:ARG:HH21	2.32	0.47
1:F:271:GLY:O	1:F:272:THR:HB	2.14	0.47
1:B:149:VAL:HA	1:B:466:MET:HE3	1.96	0.47
1:B:424:ASP:O	1:B:430:LYS:HE3	2.14	0.47
1:C:36:CYS:HA	1:C:69:TRP:O	2.15	0.47
$1:C:250:TY\overline{R:HE1}$	1:C:255:THR:CG2	2.28	0.47



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:522:TRP:CZ3	1:E:533:ILE:HD11	2.50	0.47
1:F:214:THR:HG22	1:F:215:PRO:HD2	1.97	0.47
1:G:134:ARG:NH1	1:G:300:ASP:HA	2.28	0.47
1:A:196:GLY:HA2	1:A:478:HIS:CD2	2.50	0.47
1:C:5:THR:O	1:C:8:ASP:HB2	2.14	0.47
1:C:97:ASP:HB3	1:C:100:ALA:HB2	1.97	0.47
1:C:334:ILE:O	1:C:338:LYS:HG3	2.15	0.47
1:D:131:MET:SD	1:D:298:HIS:HB3	2.54	0.47
1:F:105:PRO:HG3	1:F:210:PHE:CZ	2.50	0.47
1:B:380:ASN:HB2	1:B:417:TYR:HB3	1.96	0.46
1:D:97:ASP:HB3	1:D:100:ALA:HB2	1.97	0.46
1:D:267:HIS:CG	1:D:268:PRO:HD2	2.50	0.46
1:F:222:ILE:HG21	1:F:297:TYR:O	2.15	0.46
1:G:96:THR:HG22	1:G:246:GLN:O	2.15	0.46
1:H:437:MET:HG3	1:H:447:ASN:HB2	1.97	0.46
1:G:474:HIS:ND1	1:G:475:GLU:N	2.63	0.46
1:G:484:TRP:O	1:G:487:LEU:HB2	2.14	0.46
1:H:235:ASP:OD1	1:H:303:ARG:HD3	2.15	0.46
1:B:437:MET:CE	1:B:447:ASN:HB3	2.43	0.46
1:E:153:SER:CB	1:E:476:TRP:HE1	2.29	0.46
1:F:355:ALA:HB2	1:F:375:PHE:CD2	2.51	0.46
1:G:584:MET:HE2	1:G:609:PRO:HA	1.97	0.46
1:H:17:PHE:H	1:H:284:ASN:ND2	2.13	0.46
1:A:40:PRO:HA	1:A:67:GLY:HA2	1.98	0.46
1:B:170:GLU:HB3	1:B:171:PRO:HD3	1.98	0.46
1:E:431:GLY:O	1:E:436:LYS:NZ	2.46	0.46
1:B:403:ASP:OD2	1:F:329:GLU:OE2	2.33	0.46
1:C:267:HIS:O	1:C:271:GLY:N	2.48	0.46
1:H:560:VAL:HA	1:H:598:HIS:CE1	2.51	0.46
1:A:366:ALA:HB3	1:A:372:GLY:HA3	1.98	0.46
1:H:153:SER:CB	1:H:476:TRP:HE1	2.29	0.46
1:B:489:GLN:HB2	1:B:492:HIS:HD2	1.81	0.46
1:D:510:PRO:HA	1:D:513:TRP:CG	2.51	0.46
1:E:61:LEU:N	1:E:61:LEU:HD23	2.31	0.46
1:F:97:ASP:HB3	1:F:100:ALA:HB2	1.97	0.46
1:F:433:LEU:HA	1:F:436:LYS:HD2	1.98	0.46
1:G:62:GLU:HG3	1:G:64:TYR:CE1	2.46	0.46
1:E:236:TRP:HB2	1:E:302:LEU:HD22	1.97	0.46
1:D:165:TYR:O	1:D:168:ILE:HG22	2.16	0.46
1:F:153:SER:CB	1:F:476:TRP:HE1	2.29	0.46
1:C:12:TRP:CE2	1:C:68:LEU:HD21	2.51	0.46



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:35:PHE:CE2	1:E:47:VAL:HG11	2.51	0.46
1:H:426:VAL:HG12	1:H:476:TRP:H	1.80	0.46
1:H:573:ASN:HB3	1:H:576:ALA:HB2	1.98	0.46
1:C:49:GLY:HA2	1:C:54:TRP:CZ3	2.51	0.45
1:F:391:MET:O	1:F:438:PRO:HD3	2.16	0.45
1:G:12:TRP:HA	1:G:284:ASN:ND2	2.31	0.45
1:H:103:MET:HB3	1:H:114:LEU:HD22	1.97	0.45
1:A:312:TYR:OH	1:A:359:THR:HG21	2.16	0.45
1:C:20:SER:HB2	1:C:24:LEU:CD1	2.46	0.45
1:C:105:PRO:HB3	1:C:113:GLY:O	2.16	0.45
1:C:128:ASP:O	1:C:132:GLN:HG3	2.17	0.45
1:D:258:GLU:O	1:D:279:LYS:NZ	2.49	0.45
1:D:419:LEU:HD11	1:D:458:HIS:HB3	1.97	0.45
1:E:534:CYS:HA	1:E:546:PHE:O	2.16	0.45
1:F:472:GLN:HG2	1:F:473:HIS:N	2.30	0.45
1:G:29:ASP:OD1	1:G:72:TYR:CE1	2.67	0.45
1:B:28:PRO:HG3	1:B:118:ILE:CG2	2.47	0.45
1:D:123:TYR:OH	1:D:220:TYR:HA	2.16	0.45
1:F:460:GLY:H	1:F:515:ASP:CG	2.18	0.45
1:A:523:ILE:HB	1:A:534:CYS:HB2	1.99	0.45
1:C:469:GLU:O	1:C:495:ILE:HG22	2.17	0.45
1:D:192:HIS:CG	1:D:199:GLY:HA2	2.51	0.45
1:E:312:TYR:HE2	1:E:359:THR:HG21	1.81	0.45
1:A:165:TYR:HB2	1:A:217:ASP:HB3	1.99	0.45
1:A:173:ALA:O	1:A:177:GLN:HG3	2.15	0.45
1:A:480:THR:HG22	1:A:481:GLN:O	2.17	0.45
1:B:2:SER:OG	1:B:3:TRP:N	2.47	0.45
1:C:574:SER:HB3	1:C:613:ILE:HG23	1.97	0.45
1:E:166:ARG:HD2	1:E:220:TYR:CD2	2.52	0.45
1:F:48:LEU:HD12	1:F:83:LYS:HD3	1.97	0.45
1:F:189:ILE:HD12	1:F:218:LEU:HD21	1.97	0.45
1:F:345:TYR:OH	1:F:376:LEU:HB2	2.16	0.45
1:F:448:LEU:HD23	1:F:448:LEU:HA	1.76	0.45
1:H:419:LEU:HD11	1:H:458:HIS:HB3	1.98	0.45
1:B:17:PHE:N	1:B:284:ASN:OD1	2.49	0.45
1:E:191:GLU:OE2	1:E:210:PHE:HD1	1.99	0.45
1:E:423:HIS:HB2	1:E:476:TRP:CE3	2.52	0.45
1:E:426:VAL:O	1:E:475:GLU:HB3	2.17	0.45
1:H:391:MET:SD	1:H:550:PHE:HE2	2.39	0.45
1:A:83:LYS:HD2	1:A:94:ASP:HB3	1.99	0.45
1:A:191:GLU:OE2	1:A:209:THR:HA	2.16	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:536:LEU:HD21	1:B:563:PRO:HG2	1.99	0.45
1:B:601:PRO:HB2	1:B:602:PHE:CD1	2.52	0.45
1:F:196:GLY:HA2	1:F:478:HIS:NE2	2.31	0.45
1:H:145:SER:N	1:H:182:THR:HG22	2.20	0.45
1:H:418:ILE:HG12	1:H:461:LYS:HB2	1.99	0.45
1:A:355:ALA:HB2	1:A:375:PHE:CE1	2.52	0.45
1:D:40:PRO:O	1:D:63:ARG:NH2	2.49	0.45
1:H:551:THR:OG1	1:H:552:PRO:HD2	2.16	0.45
1:A:18:TYR:HB3	1:A:291:LEU:HD12	1.98	0.45
1:C:559:ARG:HA	1:C:604:LEU:O	2.16	0.45
1:D:433:LEU:HB3	1:D:448:LEU:HD11	1.99	0.45
1:D:570:GLU:H	1:D:588:GLY:HA2	1.82	0.45
1:F:608:LEU:HA	1:F:609:PRO:HD3	1.79	0.45
1:H:487:LEU:HA	1:H:487:LEU:HD23	1.67	0.45
1:C:345:TYR:OH	1:C:376:LEU:HB2	2.16	0.45
1:F:82:TYR:CE1	1:F:116:SER:HB3	2.51	0.45
1:F:250:TYR:CA	1:F:258:GLU:OE2	2.65	0.45
1:A:532:VAL:HG13	1:A:548:LEU:O	2.17	0.44
1:D:48:LEU:HD13	1:D:54:TRP:O	2.16	0.44
1:D:234:LEU:CD1	1:D:299:VAL:HG21	2.47	0.44
1:H:149:VAL:HA	1:H:466:MET:HE3	1.98	0.44
1:A:153:SER:CB	1:A:476:TRP:HE1	2.29	0.44
1:D:330:ASN:O	1:D:334:ILE:HG13	2.17	0.44
1:A:185:GLU:HG3	1:A:233:ILE:HB	1.99	0.44
1:D:179:LEU:HD11	1:D:469:GLU:HG3	2.00	0.44
1:E:474:HIS:NE2	1:E:483:GLU:OE2	2.51	0.44
1:A:12:TRP:HA	1:A:284:ASN:ND2	2.33	0.44
1:B:107:THR:CG2	1:D:490:PRO:HB3	2.46	0.44
1:B:523:ILE:HD11	1:B:536:LEU:HB2	2.00	0.44
1:C:431:GLY:O	1:C:436:LYS:HE2	2.17	0.44
1:F:510:PRO:HA	1:F:513:TRP:CG	2.52	0.44
1:G:154:TRP:HE3	1:G:168:ILE:HD11	1.82	0.44
1:G:449:ARG:HD2	1:G:579:TYR:HB3	1.99	0.44
1:G:465:PHE:CE1	1:G:466:MET:HG3	2.52	0.44
1:G:546:PHE:HB3	1:G:548:LEU:HD11	1.99	0.44
1:H:154:TRP:CZ3	1:H:155:ARG:HD2	2.53	0.44
1:H:189:ILE:HD12	1:H:190:MET:N	2.33	0.44
1:H:472:GLN:HG3	1:H:483:GLU:HG3	1.98	0.44
1:B:12:TRP:HA	1:B:284:ASN:HD21	1.83	0.44
1:C:35:PHE:O	1:C:70:ALA:HA	2.16	0.44
1:C:592:ALA:HA	1:C:604:LEU:HD23	1.98	0.44



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:391:MET:CE	1:D:451:LEU:HB2	2.48	0.44
1:F:28:PRO:HG3	1:F:118:ILE:HG23	1.99	0.44
1:H:351:ALA:C	1:H:352:ILE:HG13	2.38	0.44
1:H:521:GLU:OE1	1:H:600:ARG:NH1	2.37	0.44
1:A:538:LYS:HE3	1:A:538:LYS:HB2	1.88	0.44
1:C:510:PRO:HA	1:C:513:TRP:CD2	2.52	0.44
1:E:330:ASN:OD1	1:E:332:GLU:HB2	2.17	0.44
1:E:534:CYS:SG	1:E:547:VAL:HG13	2.58	0.44
1:F:241:PHE:HE1	1:F:249:VAL:HG22	1.83	0.44
1:F:484:TRP:O	1:F:487:LEU:HB2	2.16	0.44
1:C:601:PRO:HB2	1:C:602:PHE:CD1	2.52	0.44
1:D:103:MET:O	1:D:210:PHE:HB3	2.18	0.44
1:E:507:ARG:NH2	2:E:703:HOH:O	2.51	0.44
1:G:35:PHE:HZ	1:G:118:ILE:HD11	1.83	0.44
1:B:461:LYS:C	1:B:462:LYS:HD3	2.38	0.44
1:D:432:SER:O	1:D:436:LYS:HG3	2.18	0.44
1:D:604:LEU:HD23	1:D:606:LEU:HD21	2.00	0.44
1:H:469:GLU:H	1:H:469:GLU:CD	2.11	0.44
1:A:49:GLY:HA2	1:A:54:TRP:CZ3	2.53	0.44
1:B:88:HIS:CE1	1:B:254:THR:HG22	2.53	0.44
1:D:378:LYS:HD3	1:D:417:TYR:CE1	2.53	0.44
1:D:425:GLU:O	1:D:436:LYS:NZ	2.50	0.44
1:E:244:ASP:OD1	1:E:245:PRO:HD2	2.17	0.44
1:E:246:GLN:CD	1:E:246:GLN:H	2.19	0.44
1:G:28:PRO:HG3	1:G:118:ILE:HG22	2.00	0.44
1:G:482:LEU:O	1:G:484:TRP:CD1	2.70	0.44
1:B:459:PRO:HA	1:B:537:ARG:NH2	2.32	0.43
1:F:364:VAL:HG13	1:F:373:LEU:HD12	1.99	0.43
1:G:8:ASP:O	1:G:9:ILE:C	2.56	0.43
1:A:568:TRP:CD1	1:A:604:LEU:HD21	2.53	0.43
1:D:35:PHE:CD2	1:D:47:VAL:HG21	2.53	0.43
1:D:151:LEU:HD22	1:D:168:ILE:CD1	2.48	0.43
1:E:135:LYS:HD3	1:E:138:ALA:HB3	1.99	0.43
1:E:270:TRP:HD1	1:E:274:VAL:HG22	1.83	0.43
1:E:522:TRP:HH2	1:E:533:ILE:HD11	1.80	0.43
1:G:331:LEU:O	1:G:332:GLU:C	2.55	0.43
1:G:544:LEU:HB3	1:G:546:PHE:HE1	1.83	0.43
1:H:29:ASP:OD1	1:H:31:GLU:N	2.48	0.43
1:H:568:TRP:CZ3	1:H:618:PRO:HD3	2.53	0.43
1:C:548:LEU:HG	1:C:613:ILE:HD12	1.99	0.43
1:D:136:GLY:H	1:D:139:SER:HB3	1.82	0.43



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:440:ASP:OD2	1:E:440:ASP:C	2.56	0.43
1:E:453:GLY:HA3	1:E:613:ILE:HG21	2.00	0.43
1:G:49:GLY:HA2	1:G:54:TRP:CZ3	2.54	0.43
1:G:332:GLU:H	1:G:332:GLU:HG3	1.09	0.43
1:G:421:LEU:HD13	1:G:433:LEU:HD11	2.00	0.43
1:G:534:CYS:HA	1:G:546:PHE:O	2.18	0.43
1:H:536:LEU:HG	1:H:543:LEU:HD22	1.99	0.43
1:A:137:PRO:HD3	1:A:350:GLU:HA	1.99	0.43
1:A:141:TYR:O	1:A:513:TRP:HB3	2.18	0.43
1:B:19:ASP:OD1	1:B:19:ASP:N	2.50	0.43
1:D:162:SER:OG	1:D:163:PHE:N	2.52	0.43
1:D:584:MET:H	1:D:584:MET:HG2	1.45	0.43
1:F:113:GLY:O	1:F:114:LEU:HB2	2.19	0.43
1:F:596:SER:HA	1:F:600:ARG:O	2.19	0.43
1:H:151:LEU:HD11	1:H:186:LEU:HD13	1.99	0.43
1:H:193:PRO:HD3	1:H:203:VAL:CG1	2.46	0.43
1:D:59:HIS:CD2	1:D:73:VAL:HG22	2.54	0.43
1:D:564:ILE:HG22	1:D:565:GLY:O	2.17	0.43
1:E:431:GLY:N	1:E:475:GLU:OE1	2.52	0.43
1:G:331:LEU:HD13	1:G:331:LEU:HA	1.75	0.43
1:A:123:TYR:OH	1:A:220:TYR:HA	2.18	0.43
1:A:549:ASN:OD1	1:A:551:THR:HG22	2.18	0.43
1:B:48:LEU:HD11	1:B:56:PRO:HA	1.99	0.43
1:C:278:ASN:O	1:C:283:ARG:NH2	2.49	0.43
1:C:575:ASP:OD2	1:C:582:SER:HB2	2.18	0.43
1:D:276:ASP:OD1	1:D:278:ASN:HB2	2.19	0.43
1:E:95:LYS:HA	1:E:95:LYS:HD2	1.90	0.43
1:F:149:VAL:O	1:F:186:LEU:HA	2.19	0.43
1:F:403:ASP:O	1:F:407:PHE:HB2	2.19	0.43
1:F:552:PRO:O	1:F:610:PRO:HB3	2.18	0.43
1:G:149:VAL:HA	1:G:466:MET:CG	2.48	0.43
1:A:183:HIS:ND1	1:A:231:GLY:HA3	2.34	0.43
1:B:148:GLU:HB3	1:B:465:PHE:HA	2.01	0.43
1:C:101:PHE:HB2	1:C:119:THR:CG2	2.48	0.43
1:C:559:ARG:HD3	1:C:603:HIS:CE1	2.54	0.43
1:G:111:ILE:H	1:G:111:ILE:HG13	1.50	0.43
1:G:235:ASP:OD1	1:G:303:ARG:HD3	2.17	0.43
1:H:24:LEU:O	1:H:27:HIS:NE2	2.51	0.43
1:H:545:LEU:HB3	1:H:616:LEU:HB2	2.00	0.43
1:H:575:ASP:OD2	1:H:582:SER:N	2.52	0.43
1:B:552:PRO:O	1:B:610:PRO:HB3	2.17	0.43



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:155:ARG:HG2	1:C:484:TRP:HE1	1.82	0.43
1:F:562:VAL:HG21	1:F:604:LEU:HG	2.01	0.43
1:G:8:ASP:O	1:G:11:ARG:N	2.52	0.43
1:H:565:GLY:HA2	1:H:592:ALA:CB	2.49	0.43
1:B:364:VAL:HA	1:B:373:LEU:HD12	2.00	0.43
1:B:592:ALA:HB1	1:B:602:PHE:HB3	1.99	0.43
1:E:405:LEU:HD21	1:E:533:ILE:HG21	2.00	0.43
1:H:177:GLN:HG3	1:H:230:ILE:HD11	2.00	0.43
1:H:234:LEU:HG	1:H:299:VAL:HG11	2.01	0.43
1:H:293:TRP:C	1:H:299:VAL:HG22	2.39	0.43
1:A:354:ILE:HG12	1:A:377:TYR:HB2	2.00	0.43
1:A:396:VAL:O	1:A:399:LYS:HE2	2.19	0.43
1:B:3:TRP:O	1:B:23:LYS:NZ	2.36	0.43
1:B:567:PRO:HG2	1:B:619:GLU:HB3	1.99	0.43
1:C:576:ALA:HB3	1:C:579:TYR:CD2	2.54	0.43
1:C:593:VAL:O	1:C:595:GLU:N	2.44	0.43
1:E:255:THR:HG22	1:E:258:GLU:HG3	2.01	0.43
1:G:256:LEU:HD12	1:G:256:LEU:HA	1.88	0.43
1:G:571:VAL:HG21	1:G:617:GLU:HB3	2.01	0.43
1:H:85:ARG:NE	1:H:94:ASP:OD1	2.51	0.43
1:H:165:TYR:CE1	1:H:212:TYR:HB2	2.54	0.43
1:H:245:PRO:C	1:H:247:GLY:N	2.70	0.43
1:H:392:ARG:HD2	2:H:709:HOH:O	2.19	0.43
1:A:524:ASP:OD2	1:A:598:HIS:NE2	2.52	0.42
1:D:9:ILE:HG21	1:D:65:GLY:HA3	2.01	0.42
1:D:491:TYR:HD1	1:D:491:TYR:HA	1.72	0.42
1:F:254:THR:HG22	1:F:255:THR:N	2.34	0.42
1:G:143:PRO:HD3	1:G:513:TRP:CD2	2.54	0.42
1:H:222:ILE:HG12	1:H:232:VAL:HG21	2.01	0.42
1:H:241:PHE:HB3	1:H:275:PHE:CZ	2.53	0.42
1:B:392:ARG:NH2	1:B:430:LYS:O	2.52	0.42
1:B:544:LEU:HD23	1:B:544:LEU:HA	1.87	0.42
1:C:197:SER:HB2	1:C:201:GLN:HG2	2.00	0.42
1:F:96:THR:HG23	1:F:246:GLN:O	2.18	0.42
1:F:144:VAL:HB	1:F:461:LYS:HD2	2.00	0.42
1:F:514:HIS:O	1:F:537:ARG:NH1	2.48	0.42
1:A:19:ASP:CB	1:A:22:ARG:HD3	2.45	0.42
1:B:390:TYR:CE1	1:B:398:ARG:HB3	2.53	0.42
1:F:521:GLU:O	1:F:536:LEU:N	2.44	0.42
1:F:609:PRO:HA	1:F:610:PRO:HD3	1.92	0.42
1:A:426:VAL:O	1:A:426:VAL:CG1	2.68	0.42



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:28:PBO:HG3	1:B:118:ILE:HG23	2.00	0.42
1:B:146:ILE:HG21	1:B:185:GLU:HB2	2.02	0.42
1:B:241:PHE:CD2	1:B:248:LEU:HB2	2.54	0.42
1:C:49:GLY:HA3	1:C:51:PHE:CE2	2.54	0.42
1:E:570:GLU:O	1:E:570:GLU:HG3	2.20	0.42
1:F:538:LYS:O	1:F:538:LYS:HG3	2.20	0.42
1:H:165:TYR:CE2	1:H:218:LEU:HB2	2.55	0.42
1:H:256:LEU:HD12	1:H:256:LEU:HA	1.83	0.42
1:A:505:LEU:HD12	1:A:509:HIS:CE1	2.54	0.42
1:C:114:LEU:HD12	1:C:114:LEU:HA	1.83	0.42
1:C:545:LEU:O	1:C:615:ILE:HA	2.19	0.42
1:F:557:HIS:HA	1:F:605:GLU:HG3	2.02	0.42
1:G:191:GLU:OE1	1:G:209:THR:HA	2.20	0.42
1:G:399:LYS:HG3	1:G:529:ASP:HA	2.01	0.42
1:H:3:TRP:CD1	1:H:4:LEU:CD1	3.02	0.42
1:A:261:ASP:HA	1:A:262:PRO:HD3	1.94	0.42
1:A:409:LEU:HD13	1:A:409:LEU:HA	1.87	0.42
1:B:194:TYR:CZ	1:B:196:GLY:HA3	2.55	0.42
1:B:252:ASP:OD1	1:B:252:ASP:N	2.45	0.42
1:B:267:HIS:HB3	1:B:271:GLY:H	1.85	0.42
1:C:131:MET:SD	1:C:134:ARG:HD3	2.60	0.42
1:C:562:VAL:CG2	1:C:602:PHE:HB2	2.48	0.42
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.83	0.42
1:G:250:TYR:HA	1:G:254:THR:O	2.19	0.42
1:H:449:ARG:O	1:H:498:TRP:NE1	2.52	0.42
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.83	0.42
1:D:136:GLY:HA2	1:D:352:ILE:HG12	2.02	0.42
1:F:35:PHE:O	1:F:70:ALA:HA	2.20	0.42
1:F:487:LEU:HD22	1:F:493:ARG:CZ	2.50	0.42
1:A:248:LEU:HD22	1:A:248:LEU:HA	1.86	0.42
1:B:355:ALA:HB2	1:B:375:PHE:CE2	2.54	0.42
1:C:140:LEU:HD21	1:C:416:HIS:HB3	2.01	0.42
1:C:178:ASP:O	1:C:500:ARG:HG3	2.20	0.42
1:F:3:TRP:HB2	1:F:34:TRP:CZ3	2.55	0.42
1:F:192:HIS:CD2	1:F:199:GLY:HA2	2.54	0.42
1:G:36:CYS:HA	1:G:69:TRP:O	2.19	0.42
1:G:170:GLU:HB3	1:G:171:PRO:HD3	2.02	0.42
1:G:554:PRO:HB3	1:G:584:MET:HE1	2.01	0.42
1:A:278:ASN:CG	1:A:332:GLU:HG2	2.39	0.42
1:B:2:SER:HG	1:B:64:TYR:HE1	1.68	0.42
1:C:179:LEU:HD21	1:C:496:GLN:HG2	2.01	0.42



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:157:LYS:HB2	1:F:157:LYS:HE3	1.93	0.42
1:G:466:MET:CB	1:G:482:LEU:HD11	2.49	0.42
1:H:190:MET:HE1	1:H:235:ASP:O	2.19	0.42
1:C:215:PRO:HB3	1:C:297:TYR:OH	2.20	0.42
1:D:165:TYR:CZ	1:D:212:TYR:HB2	2.55	0.42
1:D:241:PHE:HZ	1:D:258:GLU:HG3	1.85	0.42
1:D:301:GLY:HA2	1:D:352:ILE:O	2.20	0.42
1:D:481:GLN:HG2	1:D:482:LEU:N	2.35	0.42
1:D:538:LYS:HB2	1:D:538:LYS:HE3	1.48	0.42
1:E:82:TYR:CD2	1:E:118:ILE:HG12	2.55	0.42
1:F:278:ASN:OD1	1:F:332:GLU:HB3	2.19	0.42
1:F:503:ASN:O	1:F:507:ARG:HG3	2.19	0.42
1:H:165:TYR:O	1:H:221:LEU:HD13	2.20	0.42
1:H:165:TYR:CZ	1:H:212:TYR:HB2	2.54	0.42
1:H:355:ALA:HB2	1:H:375:PHE:CG	2.55	0.42
1:H:455:MET:HE3	1:H:455:MET:HB3	1.79	0.42
1:A:154:TRP:CE3	1:A:155:ARG:HG3	2.55	0.41
1:A:165:TYR:CE2	1:A:212:TYR:HB2	2.55	0.41
1:B:406:THR:HG22	1:B:533:ILE:HD11	2.02	0.41
1:C:596:SER:HA	1:C:600:ARG:O	2.20	0.41
1:G:258:GLU:OE2	1:G:258:GLU:N	2.50	0.41
1:A:90:PHE:CD2	1:C:83:LYS:HD3	2.55	0.41
1:A:94:ASP:HB3	1:C:91:TYR:HD1	1.86	0.41
1:B:21:TYR:O	1:B:27:HIS:NE2	2.49	0.41
1:B:215:PRO:HB3	1:B:297:TYR:OH	2.20	0.41
1:C:96:THR:HG22	1:C:246:GLN:O	2.20	0.41
1:D:378:LYS:HD3	1:D:417:TYR:HE1	1.84	0.41
1:D:574:SER:HB3	1:D:613:ILE:H	1.86	0.41
1:F:49:GLY:HA2	1:F:54:TRP:CZ3	2.55	0.41
1:H:3:TRP:HB2	1:H:34:TRP:CE3	2.55	0.41
1:H:552:PRO:O	1:H:610:PRO:HB3	2.19	0.41
1:H:564:ILE:HG13	1:H:568:TRP:CZ2	2.55	0.41
1:C:16:THR:HG22	1:C:16:THR:O	2.19	0.41
1:C:193:PRO:HD2	1:C:194:TYR:H	1.86	0.41
1:C:301:GLY:HA2	1:C:352:ILE:O	2.21	0.41
1:C:534:CYS:HA	1:C:546:PHE:O	2.20	0.41
1:D:474:HIS:ND1	1:D:483:GLU:OE1	2.53	0.41
1:E:487:LEU:HD23	1:E:487:LEU:HA	1.89	0.41
1:E:505:LEU:HD22	1:E:572:LEU:HD12	2.02	0.41
1:F:355:ALA:HB2	1:F:375:PHE:CE2	2.55	0.41
1:A:55:ASP:HB3	1:A:58:ALA:HB2	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:393:ARG:HH11	1:A:401:HIS:CE1	2.38	0.41
1:B:3:TRP:HB2	1:B:34:TRP:CZ3	2.55	0.41
1:F:145:SER:HB3	1:F:181:PHE:HA	2.01	0.41
1:F:433:LEU:HB3	1:F:448:LEU:HD21	2.03	0.41
1:A:278:ASN:OD1	1:A:332:GLU:HG2	2.21	0.41
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.85	0.41
1:C:383:TRP:CZ2	1:C:455:MET:HB2	2.55	0.41
1:D:470:PHE:CZ	1:D:484:TRP:CE3	3.09	0.41
1:E:421:LEU:HD11	1:E:451:LEU:HD21	2.01	0.41
1:G:515:ASP:OD1	1:G:537:ARG:NH2	2.53	0.41
1:H:125:TRP:CE3	1:H:298:HIS:HD2	2.39	0.41
1:H:172:LEU:O	1:H:176:VAL:HG23	2.20	0.41
1:H:456:TRP:HA	1:H:462:LYS:CE	2.43	0.41
1:H:564:ILE:H	1:H:564:ILE:HG12	1.58	0.41
1:C:456:TRP:HA	1:C:462:LYS:CE	2.45	0.41
1:E:267:HIS:NE2	1:E:309:SER:HB2	2.35	0.41
1:E:388:LEU:HD23	1:E:388:LEU:HA	1.96	0.41
1:F:87:ARG:HD3	1:F:92:GLN:OE1	2.20	0.41
1:H:101:PHE:HB2	1:H:119:THR:HG22	2.02	0.41
1:A:16:THR:HG22	1:A:16:THR:O	2.21	0.41
1:C:179:LEU:HA	1:C:500:ARG:HG3	2.03	0.41
1:C:359:THR:HG22	1:C:360:ALA:N	2.36	0.41
1:C:533:ILE:HG13	1:C:548:LEU:HD13	2.02	0.41
1:D:526:ASN:OD1	1:D:526:ASN:O	2.39	0.41
1:E:355:ALA:HB2	1:E:375:PHE:CD2	2.56	0.41
1:E:423:HIS:HB2	1:E:476:TRP:CZ3	2.55	0.41
1:G:257:PHE:O	1:G:275:PHE:HA	2.19	0.41
1:G:421:LEU:O	1:G:463:LEU:HD23	2.20	0.41
1:G:542:ARG:HD3	1:G:542:ARG:N	2.35	0.41
1:H:149:VAL:HG12	1:H:151:LEU:HD23	2.02	0.41
1:A:149:VAL:HA	1:A:466:MET:SD	2.61	0.41
1:A:426:VAL:O	1:A:426:VAL:HG12	2.21	0.41
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.90	0.41
1:F:537:ARG:O	1:F:544:LEU:N	2.50	0.41
1:G:183:HIS:CD2	1:G:231:GLY:HA3	2.56	0.41
1:H:32:GLY:N	1:H:72:TYR:OH	2.54	0.41
1:A:87:ARG:HB2	1:A:92:GLN:HG2	2.02	0.41
1:A:487:LEU:HA	1:A:487:LEU:HD23	1.77	0.41
1:B:3:TRP:CE2	1:B:23:LYS:HD3	2.55	0.41
1:B:150:HIS:HA	2:B:715:HOH:O	2.21	0.41
1:B:342:GLU:HG3	1:B:368:THR:HG21	2.03	0.41



	to ao pagoin	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:377:TYR:HB3	1:C:418:ILE:HG13	2.02	0.41
1:C:394:ASP:HB3	1:C:397:HIS:CD2	2.55	0.41
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.91	0.41
1:E:19:ASP:OD1	1:E:19:ASP:N	2.54	0.41
1:E:148:GLU:HB3	1:E:465:PHE:HD1	1.84	0.41
1:E:522:TRP:CZ3	1:E:533:ILE:HD12	2.56	0.41
1:F:150:HIS:HB2	1:F:187:LEU:HD13	2.02	0.41
1:F:330:ASN:O	1:F:334:ILE:HG13	2.20	0.41
1:F:395:PRO:CB	1:F:552:PRO:HD3	2.51	0.41
1:G:313:ARG:NH2	1:G:332:GLU:OE2	2.54	0.41
1:G:365:SER:O	1:G:365:SER:OG	2.35	0.41
1:G:419:LEU:N	1:G:461:LYS:O	2.37	0.41
1:G:570:GLU:OE2	1:G:586:ASN:HB2	2.21	0.41
1:G:575:ASP:OD2	1:G:582:SER:HB3	2.21	0.41
1:G:584:MET:HE3	1:G:584:MET:HB3	1.77	0.41
1:H:142:GLU:O	1:H:461:LYS:NZ	2.50	0.41
1:H:434:TRP:CA	1:H:448:LEU:HD11	2.49	0.41
1:A:481:GLN:NE2	2:A:702:HOH:O	2.53	0.41
1:A:610:PRO:O	1:A:611:LEU:C	2.59	0.41
1:B:332:GLU:H	1:B:332:GLU:HG3	1.43	0.41
1:B:555:ARG:HG3	1:B:555:ARG:HH11	1.86	0.41
1:C:75:GLY:O	1:C:77:LEU:HG	2.21	0.41
1:F:44:ALA:HB3	1:F:87:ARG:HB3	2.03	0.41
1:F:280:PRO:O	1:F:284:ASN:ND2	2.54	0.41
1:H:437:MET:CG	1:H:447:ASN:HB3	2.48	0.41
1:H:524:ASP:OD2	1:H:598:HIS:NE2	2.54	0.41
1:A:34:TRP:CZ3	1:A:72:TYR:HB2	2.57	0.40
1:D:6:GLU:OE1	1:D:6:GLU:N	2.42	0.40
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.78	0.40
1:E:105:PRO:HA	1:E:114:LEU:H	1.85	0.40
1:E:572:LEU:HD12	1:E:615:ILE:HD12	2.02	0.40
1:F:201:GLN:C	1:F:242:ALA:HB2	2.42	0.40
1:F:311:LEU:HD13	1:F:361:TRP:CE3	2.56	0.40
1:H:301:GLY:HA2	1:H:352:ILE:O	2.21	0.40
1:A:176:VAL:HG13	1:A:181:PHE:HB2	2.03	0.40
1:A:571:VAL:HG21	1:A:617:GLU:HB2	2.02	0.40
1:A:571:VAL:CG2	1:A:617:GLU:HB2	2.52	0.40
1:B:19:ASP:OD2	1:B:22:ARG:CZ	2.70	0.40
1:B:30:GLU:H	1:B:30:GLU:HG2	1.44	0.40
1:B:442:TRP:HH2	1:B:610:PRO:HB2	1.86	0.40
1:D:596:SER:HA	1:D:600:ARG:O	2.21	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:F:311:LEU:HD13	1:F:361:TRP:CD2	2.56	0.40
1:G:176:VAL:HG13	1:G:181:PHE:HB2	2.03	0.40
1:A:125:TRP:HB3	1:A:127:ASP:OD1	2.21	0.40
1:A:552:PRO:O	1:A:610:PRO:HB3	2.21	0.40
1:A:576:ALA:HB3	1:A:579:TYR:CD2	2.56	0.40
1:B:192:HIS:CD2	1:B:199:GLY:HA2	2.56	0.40
1:B:456:TRP:HA	1:B:462:LYS:HE3	2.03	0.40
1:C:354:ILE:HG12	1:C:377:TYR:HB2	2.03	0.40
1:C:572:LEU:HD23	1:C:572:LEU:HA	1.96	0.40
1:D:16:THR:O	1:D:16:THR:HG22	2.21	0.40
1:A:188:PRO:HG3	1:A:235:ASP:HB3	2.03	0.40
1:B:512:LEU:HD23	1:B:537:ARG:HG2	2.04	0.40
1:D:68:LEU:HD23	1:D:68:LEU:HA	1.92	0.40
1:G:136:GLY:HA3	1:G:137:PRO:HD3	1.95	0.40
1:G:597:TRP:HB2	1:G:603:HIS:HB3	2.02	0.40
1:H:170:GLU:HA	1:H:224:TYR:HE2	1.87	0.40
1:H:523:ILE:HD11	1:H:536:LEU:HD13	2.04	0.40
1:A:601:PRO:HB2	1:A:602:PHE:CD1	2.56	0.40
1:B:191:GLU:OE1	1:B:209:THR:HA	2.22	0.40
1:B:393:ARG:HE	1:B:401:HIS:CD2	2.39	0.40
1:C:571:VAL:HG22	1:C:615:ILE:O	2.21	0.40
1:D:49:GLY:HA3	1:D:51:PHE:CE1	2.56	0.40
1:D:143:PRO:HD3	1:D:513:TRP:CE2	2.57	0.40
1:E:105:PRO:HG3	1:E:210:PHE:CE2	2.56	0.40
1:E:365:SER:HA	1:E:375:PHE:O	2.22	0.40
1:F:310:MET:HE2	1:F:310:MET:HB3	1.92	0.40
1:G:12:TRP:HA	1:G:284:ASN:HD21	1.86	0.40
1:G:105:PRO:HA	1:G:106:PRO:HD3	1.90	0.40
1:H:28:PRO:HA	1:H:33:THR:HG22	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	Percentiles
1	А	597/620~(96%)	577~(97%)	19 (3%)	1 (0%)	44 72
1	В	599/620~(97%)	$580 \ (97\%)$	18 (3%)	1 (0%)	44 72
1	С	602/620~(97%)	582 (97%)	19 (3%)	1 (0%)	44 72
1	D	593/620~(96%)	571 (96%)	21~(4%)	1 (0%)	44 72
1	Е	598/620~(96%)	576~(96%)	21~(4%)	1 (0%)	44 72
1	F	587/620~(95%)	558~(95%)	28~(5%)	1 (0%)	44 72
1	G	600/620~(97%)	576 (96%)	23~(4%)	1 (0%)	44 72
1	Н	597/620~(96%)	582 (98%)	14 (2%)	1 (0%)	44 72
All	All	4773/4960 (96%)	4602 (96%)	163 (3%)	8 (0%)	44 72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	420	PRO
1	В	420	PRO
1	Е	420	PRO
1	F	420	PRO
1	Н	420	PRO
1	D	420	PRO
1	С	420	PRO
1	G	420	PRO

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	490/528~(93%)	464 (95%)	26~(5%)	19	48
1	В	497/528~(94%)	476 (96%)	21 (4%)	25	57
1	С	496/528~(94%)	468 (94%)	28~(6%)	17	46
1	D	494/528~(94%)	464 (94%)	30~(6%)	15	42
1	Е	496/528~(94%)	477 (96%)	19 (4%)	28	61
1	F	494/528~(94%)	465 (94%)	29(6%)	16	43



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	494/528~(94%)	467 (94%)	27~(6%)	18	46
1	Н	472/528~(89%)	443 (94%)	29 (6%)	15	42
All	All	3933/4224 (93%)	3724 (95%)	209 (5%)	19	48

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	17	PHE
1	А	24	LEU
1	А	29	ASP
1	А	61	LEU
1	А	77	LEU
1	А	85	ARG
1	А	107	THR
1	А	120	ARG
1	А	145	SER
1	А	178	ASP
1	А	190	MET
1	А	248	LEU
1	А	270	TRP
1	А	340	PHE
1	А	350	GLU
1	А	419	LEU
1	А	422	SER
1	А	432	SER
1	А	463	LEU
1	А	474	HIS
1	А	496	GLN
1	А	538	LYS
1	А	543	LEU
1	А	556	GLU
1	А	558	TYR
1	А	613	ILE
1	В	13	GLU
1	В	17	PHE
1	В	29	ASP
1	В	30	GLU
1	В	109	SER
1	В	111	ILE
1	В	114	LEU
1	В	122	ASP



Mol	Chain	Res	Type
1	В	134	ARG
1	В	153	SER
1	В	190	MET
1	В	331	LEU
1	В	332	GLU
1	В	353	THR
1	В	394	ASP
1	В	424	ASP
1	В	537	ARG
1	В	541	ASP
1	В	542	ARG
1	В	555	ARG
1	В	587	PHE
1	С	2	SER
1	С	17	PHE
1	С	19	ASP
1	С	24	LEU
1	С	107	THR
1	С	109	SER
1	С	111	ILE
1	С	114	LEU
1	С	134	ARG
1	С	135	LYS
1	С	172	LEU
1	С	184	VAL
1	С	261	ASP
1	С	264	MET
1	С	274	VAL
1	С	314	ASP
1	C	332	GLU
1	С	358	SER
1	С	414	SER
1	C	422	SER
1	C	528	ARG
1	C	537	ARG
1	C	538	LYS
1	C	543	LEU
1	C	551	THR
1	C	582	SER
1	С	586	ASN
1	C	613	ILE
1	D	14	SER



Mol	Chain	Res	Type
1	D	17	PHE
1	D	29	ASP
1	D	51	PHE
1	D	87	ARG
1	D	114	LEU
1	D	145	SER
1	D	164	SER
1	D	179	LEU
1	D	190	MET
1	D	214	THR
1	D	270	TRP
1	D	274	VAL
1	D	313	ARG
1	D	339	LYS
1	D	409	LEU
1	D	414	SER
1	D	421	LEU
1	D	422	SER
1	D	451	LEU
1	D	470	PHE
1	D	480	THR
1	D	483	GLU
1	D	518	GLU
1	D	543	LEU
1	D	559	ARG
1	D	582	SER
1	D	584	MET
1	D	590	VAL
1	D	605	GLU
1	Е	14	SER
1	Е	17	PHE
1	E	107	THR
1	Е	120	ARG
1	Е	155	ARG
1	E	157	LYS
1	Е	164	SER
1	Е	209	THR
1	E	246	GLN
1	E	270	TRP
1	E	314	ASP
1	Е	332	GLU
1	E	394	ASP



Mol	Chain	Res	Type
1	Е	399	LYS
1	Е	409	LEU
1	Е	470	PHE
1	Е	542	ARG
1	Е	569	ARG
1	Е	613	ILE
1	F	17	PHE
1	F	29	ASP
1	F	122	ASP
1	F	128	ASP
1	F	134	ARG
1	F	190	MET
1	F	214	THR
1	F	258	GLU
1	F	303	ARG
1	F	332	GLU
1	F	335	ASP
1	F	392	ARG
1	F	393	ARG
1	F	421	LEU
1	F	422	SER
1	F	425	GLU
1	F	448	LEU
1	F	451	LEU
1	F	455	MET
1	F	462	LYS
1	F	463	LEU
1	F	479	ASP
1	F	$52\overline{4}$	ASP
1	F	543	LEU
1	F	556	GLU
1	F	562	VAL
1	F	605	GLU
1	F	613	ILE
1	F	614	LEU
1	G	17	PHE
1	G	24	LEU
1	G	53	ASN
1	G	107	THR
1	G	111	ILE
1	G	114	LEU
1	G	120	ARG



Mol	Chain	Res	Type
1	G	161	VAL
1	G	162	SER
1	G	270	TRP
1	G	314	ASP
1	G	331	LEU
1	G	332	GLU
1	G	339	LYS
1	G	347	HIS
1	G	365	SER
1	G	394	ASP
1	G	432	SER
1	G	455	MET
1	G	462	LYS
1	G	474	HIS
1	G	522	TRP
1	G	526	ASN
1	G	541	ASP
1	G	558	TYR
1	G	607	THR
1	G	617	GLU
1	Н	2	SER
1	Н	5	THR
1	Н	17	PHE
1	Н	21	TYR
1	Н	29	ASP
1	Н	47	VAL
1	Н	55	ASP
1	Н	60	GLN
1	Н	62	GLU
1	Н	63	ARG
1	Н	85	ARG
1	Н	95	LYS
1	H	114	LEU
1	Н	201	GLN
1	Η	202	VAL
1	Н	246	GLN
1	Н	254	THR
1	H	270	TRP
1	Н	278	ASN
1	Н	299	VAL
1	Н	391	MET
1	Н	403	ASP



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Mol	Chain	Res	Type
1	Н	408	SER
1	Н	472	GLN
1	Н	496	GLN
1	Н	505	LEU
1	Н	562	VAL
1	Н	590	VAL
1	Н	617	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	59	HIS
1	А	177	GLN
1	В	330	ASN
1	В	370	ASN
1	С	474	HIS
1	С	492	HIS
1	D	267	HIS
1	D	278	ASN
1	D	347	HIS
1	D	489	GLN
1	D	509	HIS
1	Е	246	GLN
1	Е	539	HIS
1	F	385	HIS
1	F	496	GLN
1	G	385	HIS
1	G	492	HIS
1	Н	60	GLN
1	Н	472	GLN
1	Н	526	ASN
1	Н	530	GLN

#### 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 oligosaccharides 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	$OWAB(Å^2)$	Q < 0.9
1	А	603/620~(97%)	-0.15	13 (2%) 62 56	19, 34, 56, 109	0
1	В	603/620~(97%)	-0.20	11 (1%) 67 62	17, 33, 54, 103	0
1	С	606/620~(97%)	-0.23	14 (2%) 61 55	18, 33, 60, 100	0
1	D	599/620~(96%)	-0.13	9 (1%) 71 66	22, 36, 57, 93	0
1	Е	604/620~(97%)	-0.15	12 (1%) 64 58	21, 38, 60, 95	0
1	F	593/620~(95%)	-0.18	11 (1%) 66 60	20, 35, 54, 79	0
1	G	606/620~(97%)	-0.01	10 (1%) 69 63	22, 39, 64, 100	0
1	Н	$60\overline{3}/620~(97\%)$	0.36	31 (5%) 34 29	25, 48, 73, 88	0
All	All	4817/4960 (97%)	-0.09	111 (2%) 61 55	17, 37, 63, 109	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	420	PRO	5.3
1	G	326	GLY	5.0
1	А	272	THR	4.5
1	С	266	HIS	4.3
1	Н	585	GLY	4.2
1	F	271	GLY	4.1
1	G	325	PHE	4.1
1	G	529	ASP	4.1
1	Н	266	HIS	4.0
1	С	265	ARG	3.9
1	Н	529	ASP	3.8
1	D	272	THR	3.6
1	D	420	PRO	3.5
1	Е	587	PHE	3.5
1	F	420	PRO	3.5
1	В	313	ARG	3.5



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Mol	Chain	Res	Type	RSRZ
1	А	324	ILE	3.5
1	А	420	PRO	3.4
1	Н	489	GLN	3.4
1	D	267	HIS	3.4
1	В	587	PHE	3.3
1	Е	158	GLN	3.3
1	G	420	PRO	3.2
1	Н	401	HIS	3.2
1	F	30	GLU	3.2
1	Е	271	GLY	3.2
1	Н	587	PHE	3.1
1	Н	588	GLY	3.1
1	С	588	GLY	3.0
1	С	264	MET	3.0
1	Н	267	HIS	2.9
1	G	551	THR	2.9
1	Н	619	GLU	2.9
1	С	262	PRO	2.9
1	В	266	HIS	2.9
1	F	524	ASP	2.9
1	Н	19	ASP	2.9
1	Н	271	GLY	2.9
1	F	272	THR	2.9
1	Н	550	PHE	2.8
1	А	64	TYR	2.8
1	С	420	PRO	2.8
1	В	265	ARG	2.8
1	Н	265	ARG	2.8
1	А	325	PHE	2.8
1	В	110	PRO	2.7
1	С	586	ASN	2.7
1	Н	162	SER	2.7
1	Е	262	PRO	2.7
1	А	270	TRP	2.7
1	В	261	ASP	2.7
1	D	273	TYR	2.7
1	Е	268	PRO	2.6
1	G	421	LEU	2.6
1	Н	420	PRO	2.6
1	Н	589	ARG	2.6
1	С	111	ILE	2.6
1	Е	270	TRP	2.6



Mol	Chain	Res	Type	RSRZ
1	С	272	THR	2.6
1	С	268	PRO	2.5
1	F	619	GLU	2.5
1	А	66	ALA	2.5
1	G	107	THR	2.5
1	F	556	GLU	2.4
1	В	423	HIS	2.4
1	А	63	ARG	2.4
1	А	271	GLY	2.3
1	Н	500	ARG	2.3
1	В	264	MET	2.3
1	Е	588	GLY	2.3
1	Н	108	GLY	2.3
1	D	270	TRP	2.3
1	F	2	SER	2.3
1	D	214	THR	2.3
1	Н	272	THR	2.3
1	Н	400	TYR	2.3
1	Н	581	GLY	2.3
1	G	587	PHE	2.3
1	Е	269	ASP	2.3
1	Н	109	SER	2.3
1	С	359	THR	2.3
1	Е	526	ASN	2.2
1	G	530	GLN	2.2
1	С	587	PHE	2.2
1	F	31	GLU	2.2
1	G	619	GLU	2.2
1	Н	167	GLU	2.2
1	D	268	PRO	2.2
1	A	526	ASN	2.2
1	Е	533	ILE	2.2
1	Η	474	HIS	2.2
1	F	543	LEU	2.2
1	А	245	PRO	2.2
1	Н	582	SER	2.2
1	А	327	GLY	2.1
1	В	107	THR	2.1
1	Н	442	TRP	2.1
1	Η	268	PRO	2.1
1	F	29	ASP	2.1
1	Н	590	VAL	2.1



Mol	Chain	Res	Type	RSRZ
1	В	589	ARG	2.1
1	Е	420	PRO	2.1
1	А	65	GLY	2.1
1	Н	23	LYS	2.1
1	С	263	ARG	2.1
1	Е	470	PHE	2.1
1	D	269	ASP	2.0
1	Н	128	ASP	2.0
1	Н	224	TYR	2.0
1	D	584	MET	2.0
1	С	270	TRP	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.

