

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 03:23 PM JST

PDB ID	:	8GPU
Title	:	$YFV_E_YD6Fab_prefusion$
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Deposited on	:	2022-08-27
Resolution	:	2.79 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:

:	4.02b-467
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	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 2.79 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.



Motria	Whole archive	Similar resolution
	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	А	398	78%	20%	••
1	В	398	72%	23%	••
1	Е	398	74%	23%	•••
1	Ι	398	80%	16%	
1	М	398	76%	21%	•••
1	Р	398	78%	18%	••
2	С	217	70%	27%	•
2	F	217	88%	1	2%



Mol	Chain	Length	Quality of chain		
2	Н	217	80%	18%	•
2	J	217	72%	23%	••
2	Ν	217	75%	24%	•
2	Q	217	81%	18%	
3	D	217	72%	24%	••
3	G	217	83%	15%	•
3	K	217	76%	20%	••
3	L	217	71%	26%	•••
3	0	217	80%	17%	•••
3	R	217	76%	19%	•••



$8 \mathrm{GPU}$

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	A 200	Total	С	Ν	0	\mathbf{S}	0	1	0
	A	592	2997	1877	518	582	20	0	L	0
1	F	300	Total	С	Ν	0	S	0	0	0
1	Ľ	592	2985	1868	515	582	20	0	0	0
1	В	200	Total	С	Ν	0	S	0	1	0
1	D	300	2965	1861	512	572	20	0		0
1	т	388	Total	С	Ν	0	S	0	0	0
1	1	300	2952	1853	508	571	20	0	0	
1	М	388	Total	С	Ν	0	S	0	0	0
1	1 1/1	300	2950	1851	508	571	20	0	0	0
1	1 P	388	Total	С	Ν	Ο	S	0	0	0
			2950	1851	508	571	20	0	U	U

• Molecule 1 is a protein called Envelope protein.

• Molecule 2 is a protein called YD6Fab_H.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace	
0	<u>а п</u>	916	Total	С	Ν	0	S	0	0	0	
	11	210	1623	1028	270	318	$\overline{7}$	0	0	0	
0	Б	216	Total	С	Ν	0	S	0	0	0	
	Г	210	1623	1028	270	318	7	0	0	0	
2	С	C	216	Total	С	Ν	0	S	0	0	0
	U	210	1623	1028	270	318	$\overline{7}$	0	0	0	
0	т	911	Total	С	Ν	0	S	0	0	0	
	J	211	1591	1010	264	310	7	0	0		
0	N	216	Total	С	Ν	0	S	0	0	0	
2 IN	210	1623	1028	270	318	7	0	0	0		
2	2 0	916	Total	С	Ν	Ο	S	0	0	0	
	V V	210	1623	1028	270	318	7	0	0	U	

• Molecule 3 is a protein called YD6Fab_L.



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	о т	214	Total	С	Ν	0	\mathbf{S}	0	0	0
0		214	1601	1004	267	325	5	0	0	0
3	С	216	Total	С	Ν	0	S	0	0	0
0	G	210	1614	1010	268	330	6	0	0	0
3	Л	213	Total	С	Ν	0	S	0	0	0
0	D		1594	1000	266	323	5	0	0	0
3	K	914	Total	С	Ν	0	S	0	0	0
0	Γ	214	1601	1004	267	325	5	0	0	0
3	0	217	Total	С	Ν	0	S	0	0	0
0	3 0		1623	1015	270	332	6	0	0	0
3	В	913	Total	С	Ν	Ο	S	0	0	0
3 R	213	1594	1000	266	323	5	0	0	U	



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

• Molecule 1: Envelope protein





ILE GLY LYS

• Molecule 1: Envelope protein



F170 GLU S184 L4 V186 R19 V205 F29 M203 C22 M204 C22 M205 F29 M205 M35 M205 M36 M206 M35 M206 M35 M207 M36 M316 M36 M316 M36 M316 M36 M317 M36 M3114 M36 M3106 M36 </t

• Molecule 2: YD6Fab_H





 \bullet Molecule 3: YD6Fab_L





• Molecule 3: YD6Fab_L





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	42.57 - 2.79	Depositor
% Data completeness (in resolution range)	85.4 (42.57-2.79)	Depositor
R _{merge}	0.18	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.03 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.244 , 0.279	Depositor
Wilson B-factor $(Å^2)$	49.9	Xtriage
Anisotropy	0.138	Xtriage
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	$\begin{array}{c} 0.006 \mbox{ for } 1/2 \mbox{``h-1/2*k,-3/2*h-1/2*k,-l} \\ 0.006 \mbox{ for } 1/2 \mbox{``h+1/2*k,3/2*h-1/2*k,-l} \end{array}$	Xtriage
Total number of atoms	37132	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.78% 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).

Mal	Chain	Bond	lengths	Bo	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.28	0/3061	0.52	0/4153
1	В	0.27	0/3025	0.54	0/4102
1	Е	0.28	0/3045	0.55	2/4132~(0.0%)
1	Ι	0.26	0/3011	0.52	1/4084~(0.0%)
1	М	0.29	0/3009	0.55	1/4081~(0.0%)
1	Р	0.28	0/3009	0.54	0/4081
2	С	0.31	0/1662	0.57	0/2262
2	F	0.29	0/1662	0.55	1/2262~(0.0%)
2	Н	0.28	0/1662	0.53	0/2262
2	J	0.29	0/1629	0.56	0/2217
2	Ν	0.27	0/1662	0.56	0/2262
2	Q	0.28	0/1662	0.52	0/2262
3	D	0.30	0/1634	0.54	0/2232
3	G	0.31	0/1654	0.56	0/2258
3	Κ	0.33	0/1641	0.58	0/2242
3	L	0.33	0/1641	0.57	0/2242
3	0	0.32	0/1663	0.59	1/2270~(0.0%)
3	R	0.33	0/1634	0.55	0/2232
All	All	0.29	0/37966	0.55	6/51636~(0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1
1	Ι	0	1
3	Κ	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
3	0	114	PRO	N-CA-CB	-7.17	94.70	103.30
1	Ε	329	PRO	CA-N-CD	-6.08	102.99	111.50
1	Ι	329	PRO	CA-N-CD	-5.52	103.77	111.50
1	М	382	ASP	CB-CA-C	5.31	121.02	110.40
1	Е	329	PRO	N-CA-CB	-5.21	96.87	102.60
2	F	118	ALA	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	В	328	ALA	Mainchain
1	Ι	328	ALA	Mainchain
3	Κ	112	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2997	0	2934	54	0
1	В	2965	0	2908	77	0
1	Е	2985	0	2911	53	0
1	Ι	2952	0	2893	39	0
1	М	2950	0	2886	48	0
1	Р	2950	0	2886	56	0
2	С	1623	0	1595	46	0
2	F	1623	0	1595	15	0
2	Н	1623	0	1595	26	0
2	J	1591	0	1561	38	0
2	N	1623	0	1595	39	0
2	Q	1623	0	1595	22	0
3	D	1594	0	1541	38	0
3	G	1614	0	1553	20	0
3	K	1601	0	1548	41	0
3	L	1601	0	1548	38	0
3	0	1623	0	1564	44	0
3	R	1594	0	1541	32	0
All	All	37132	0	36249	689	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 (689) 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:P:328:ALA:CB	1:P:329:PRO:HD2	1.72	1.19
2:C:76:LYS:O	2:C:78:LEU:HD23	1.43	1.18
3:0:113:GLN:CG	3:O:114:PRO:HD3	1.76	1.14
1:P:328:ALA:HB1	1:P:329:PRO:CD	1.79	1.13
3:O:113:GLN:CB	3:O:114:PRO:HD3	1.78	1.12
1:P:328:ALA:CB	1:P:329:PRO:CD	2.25	1.12
1:A:328:ALA:HB1	1:A:329:PRO:HD2	1.16	1.10
1:P:328:ALA:HB3	1:P:329:PRO:HD2	1.30	1.06
1:B:328:ALA:HB1	1:B:329:PRO:CD	1.87	1.05
1:B:328:ALA:HB1	1:B:329:PRO:HD2	1.40	1.04
3:O:113:GLN:HG3	3:0:114:PRO:CD	1.88	1.04
3:O:113:GLN:HB2	3:O:114:PRO:HD3	1.38	1.03
3:O:20:ILE:HD11	3:O:108:LEU:CD1	1.91	0.99
3:K:113:GLN:HB2	3:K:114:PRO:HD3	1.44	0.98
1:A:328:ALA:HB1	1:A:329:PRO:CD	1.95	0.96
1:B:187:ALA:HB2	1:B:279:GLY:HA3	1.48	0.95
3:O:113:GLN:HG3	3:O:114:PRO:HD3	1.49	0.90
1:P:328:ALA:HB1	1:P:329:PRO:HD3	1.51	0.90
1:E:329:PRO:HD3	1:E:357:SER:O	1.72	0.89
1:A:328:ALA:CB	1:A:329:PRO:HD2	2.01	0.89
3:D:109:THR:HG21	3:D:146:PRO:HB3	1.55	0.87
1:P:179:THR:HB	1:P:286:LYS:HB3	1.56	0.86
1:M:303:LYS:HA	1:M:383:SER:OG	1.76	0.85
2:J:123:PRO:HB3	2:J:149:TYR:HB3	1.58	0.85
2:C:76:LYS:O	2:C:78:LEU:CD2	2.24	0.84
3:O:113:GLN:CB	3:0:114:PRO:CD	2.57	0.82
3:G:113:GLN:CG	3:G:114:PRO:HD3	2.09	0.82
3:0:113:GLN:CG	3:0:114:PRO:CD	2.50	0.82
2:H:163:LEU:HD21	2:H:186:VAL:HG21	1.61	0.81
3:K:29:ILE:HG22	3:K:68:LYS:HE3	1.62	0.80
1:B:265:THR:HG1	1:B:277:HIS:HE2	1.30	0.80
3:G:113:GLN:HG2	3:G:114:PRO:CD	2.12	0.79
1:B:328:ALA:CB	1:B:329:PRO:HD2	2.11	0.79
3:O:20:ILE:HD11	3:O:108:LEU:HD11	1.63	0.78
3:O:113:GLN:HB2	3:0:114:PRO:CD	2.15	0.77
2:N:170:PHE:HD2	3:O:180:SER:HB3	1.49	0.77
3:G:113:GLN:HG3	3:G:114:PRO:HD3	1.66	0.77



	to do pago	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:142:LEU:HD11	2:C:198:TYR:HE2	1.51	0.76
3:O:113:GLN:HG3	3:O:114:PRO:HD2	1.64	0.76
3:L:113:GLN:HB2	3:L:114:PRO:CD	2.16	0.76
2:C:167:VAL:HG22	2:C:186:VAL:HG12	1.69	0.76
1:M:323:LYS:HG3	1:M:362:GLU:HG2	1.68	0.75
3:G:113:GLN:CG	3:G:114:PRO:CD	2.64	0.75
3:G:113:GLN:HG2	3:G:114:PRO:HD2	1.69	0.74
3:L:113:GLN:HB2	3:L:114:PRO:HD3	1.71	0.73
1:E:303:LYS:HA	1:E:383:SER:HB3	1.70	0.72
1:P:95:THR:HG22	1:P:96:TYR:H	1.55	0.72
3:K:113:GLN:HB2	3:K:114:PRO:CD	2.19	0.71
2:C:127:PRO:HG3	2:C:213:LYS:HG3	1.73	0.71
3:D:113:GLN:HG2	3:D:114:PRO:HD2	1.72	0.71
3:D:113:GLN:HG2	3:D:114:PRO:CD	2.21	0.71
2:F:130:PRO:HB3	2:F:142:LEU:HD11	1.73	0.70
1:M:99:ARG:HA	1:M:103:ASN:HD21	1.58	0.69
3:K:29:ILE:O	3:K:68:LYS:NZ	2.22	0.69
3:R:172:GLN:N	3:R:176:LYS:O	2.21	0.69
1:E:304:MET:HG2	1:E:324:VAL:HG22	1.74	0.68
2:N:91:THR:HG23	2:N:114:THR:HA	1.75	0.68
3:G:32:TYR:HB3	3:G:34:LEU:HD23	1.76	0.68
2:H:98:THR:HG1	2:H:106:THR:HG1	1.40	0.68
2:Q:199:ILE:HG12	2:Q:214:ARG:HG2	1.74	0.68
2:C:142:LEU:HD13	2:C:215:VAL:HG11	1.75	0.67
1:P:146:GLY:HA3	1:P:363:VAL:HG23	1.77	0.67
3:D:29:ILE:O	3:D:31:THR:N	2.27	0.67
1:A:235:GLU:OE2	1:B:263:ARG:NH1	2.27	0.67
3:K:85:GLU:HG3	3:K:109:THR:HA	1.77	0.66
2:J:170:PHE:HE2	3:K:180:SER:HB3	1.59	0.66
3:R:53:VAL:HG11	3:R:68:LYS:HB2	1.77	0.66
2:J:175:GLN:H	2:J:175:GLN:HE21	1.42	0.65
1:M:50:ILE:HD11	1:M:190:PHE:HE2	1.62	0.65
3:O:18:ILE:HG21	3:O:108:LEU:HD21	1.78	0.65
1:P:323:LYS:HG3	1:P:362:GLU:HG2	1.77	0.65
1:B:84:GLU:OE1	1:B:84:GLU:N	2.30	0.65
1:B:328:ALA:HB1	1:B:329:PRO:HD3	1.78	0.65
1:E:171:GLU:HB3	1:E:177:LYS:HB3	1.79	0.65
1:P:130:VAL:HG11	1:P:190:PHE:CZ	2.32	0.65
3:R:32:TYR:HB3	3:R:34:LEU:HD23	1.79	0.65
1:E:267:ASP:OD2	1:E:275:LYS:NZ	2.21	0.64
1:A:179:THR:HB	1:A:286:LYS:HB3	1.77	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:O:20:ILE:CD1	3:O:108:LEU:CD1	2.70	0.64
3:G:63:ARG:NH1	3:G:79:GLY:O	2.30	0.64
3:O:139:CYS:HB3	3:0:181:SER:OG	1.98	0.64
3:G:171:LYS:HE3	3:G:175:ASN:HA	1.80	0.64
1:I:332:ILE:HB	1:I:354:PRO:HB2	1.80	0.63
3:D:34:LEU:HA	3:D:52:GLU:HA	1.79	0.63
3:D:63:ARG:NH2	3:D:84:ASP:OD2	2.30	0.63
1:M:328:ALA:HB1	1:M:329:PRO:HD2	1.80	0.63
2:N:18:LEU:HD12	2:N:19:ARG:H	1.63	0.63
2:J:64:VAL:HB	2:J:68:PHE:HD2	1.64	0.63
3:O:77:ILE:HD13	3:O:80:LEU:HD13	1.80	0.63
2:H:91:THR:HG23	2:H:114:THR:HA	1.79	0.63
2:F:91:THR:HG23	2:F:114:THR:HA	1.78	0.63
1:I:62:SER:HB3	1:I:123:LYS:HB2	1.80	0.63
1:I:329:PRO:HD3	1:I:357:SER:O	1.99	0.62
1:E:179:THR:HB	1:E:286:LYS:HB3	1.81	0.62
2:C:160:SER:HA	2:C:201:ASN:OD1	1.99	0.62
1:E:40:SER:HB2	1:E:144:HIS:HB2	1.80	0.62
3:R:113:GLN:HB3	3:R:114:PRO:CD	2.30	0.62
2:Q:143:GLY:HA3	2:Q:185:VAL:HG12	1.80	0.62
1:A:310:PRO:HD2	1:A:387:TYR:HD2	1.64	0.62
2:N:154:VAL:HG12	2:N:204:HIS:HD2	1.64	0.62
2:C:35:MET:HB3	2:C:50:TYR:HD1	1.65	0.62
2:Q:91:THR:HG23	2:Q:114:THR:HA	1.81	0.62
2:C:11:LEU:HD12	2:C:11:LEU:O	2.00	0.61
2:H:50:TYR:HB3	2:H:59:TYR:HB2	1.80	0.61
2:F:36:TRP:HD1	2:F:70:ILE:HD12	1.65	0.61
2:J:148:ASP:HA	2:J:179:LEU:HD13	1.81	0.61
3:K:185:LEU:HD22	3:K:189:GLN:HB3	1.83	0.61
1:A:84:GLU:N	1:A:84:GLU:OE1	2.31	0.61
3:L:85:GLU:HB2	3:L:110:VAL:HG22	1.83	0.61
3:L:113:GLN:CB	3:L:114:PRO:CD	2.76	0.61
1:P:206:ASP:OD1	1:P:208:GLN:N	2.34	0.61
1:E:152:TRP:O	1:E:156:ILE:HG13	2.00	0.61
3:R:174:ASN:ND2	3:R:176:LYS:HD2	2.16	0.61
3:K:109:THR:HG21	3:K:146:PRO:HB3	1.83	0.60
1:E:62:SER:HB3	1:E:123:LYS:HB2	1.83	0.60
1:E:99:ARG:HA	1:E:103:ASN:HD21	1.66	0.60
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.65	0.60
1:I:328:ALA:HB1	1:I:329:PRO:HD2	1.82	0.60
3:L:137:LEU:HD13	3:L:183:LEU:HD23	1.83	0.60



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:28:ASN:HA	3:G:94:ALA:HA	1.84	0.60
2:J:163:LEU:HD21	2:J:186:VAL:HG21	1.83	0.60
3:L:62:ASN:ND2	3:R:59:GLY:HA3	2.16	0.60
1:I:294:GLY:HA3	1:I:355:ILE:HD11	1.83	0.60
3:R:26:GLY:O	3:R:71:ASN:ND2	2.33	0.60
1:A:130:VAL:HG21	1:A:190:PHE:CE1	2.36	0.59
2:C:130:PRO:HB3	2:C:142:LEU:HB3	1.84	0.59
1:P:130:VAL:HG11	1:P:190:PHE:CE1	2.37	0.59
3:R:174:ASN:HD21	3:R:176:LYS:HD2	1.66	0.59
2:J:123:PRO:CB	2:J:149:TYR:HB3	2.32	0.59
2:N:19:ARG:NH1	2:N:82:GLN:OE1	2.35	0.59
3:D:113:GLN:CG	3:D:114:PRO:CD	2.81	0.59
3:R:95:ASP:OD1	3:R:98:ILE:HB	2.02	0.59
1:M:46:GLN:HG2	1:M:47:THR:HG23	1.82	0.59
3:O:53:VAL:HG11	3:O:68:LYS:HG3	1.85	0.59
1:A:131:ASP:HB3	1:A:134:LYS:HG3	1.83	0.59
2:N:22:CYS:HB3	2:N:79:LEU:HB3	1.85	0.59
3:L:13:SER:H	3:L:16:GLN:HE22	1.50	0.59
3:G:113:GLN:HB3	3:G:145:TYR:CE2	2.38	0.59
3:D:125:PRO:HD2	3:D:190:TRP:CZ2	2.38	0.59
3:D:156:ASP:OD1	3:D:195:SER:N	2.26	0.59
3:K:113:GLN:CB	3:K:114:PRO:CD	2.81	0.59
1:M:62:SER:HB3	1:M:123:LYS:HB2	1.84	0.59
1:E:268:GLU:O	1:E:270:ASP:N	2.29	0.58
1:B:3:CYS:HB3	1:B:9:ARG:HG3	1.85	0.58
3:O:63:ARG:NH2	3:O:84:ASP:OD2	2.35	0.58
2:C:157:SER:O	2:C:201:ASN:N	2.37	0.58
1:P:297:TYR:O	1:P:331:LYS:NZ	2.37	0.58
1:A:58:LYS:HG3	1:A:220:GLY:HA2	1.84	0.58
1:B:265:THR:OG1	1:B:277:HIS:NE2	2.23	0.58
1:M:137:TYR:CE1	1:M:184:VAL:HG22	2.39	0.58
1:B:187:ALA:HB2	1:B:279:GLY:CA	2.29	0.58
2:C:52:SER:O	2:C:72:ARG:NH1	2.37	0.58
1:A:93:LYS:HD2	1:A:234:PHE:HB2	1.85	0.58
3:G:13:SER:H	3:G:16:GLN:NE2	2.02	0.58
3:O:63:ARG:NH1	3:O:78:SER:O	2.37	0.58
2:N:87:ARG:HD3	2:N:89:GLU:OE1	2.04	0.57
1:A:369:PRO:HG2	1:A:391:LYS:HE3	1.86	0.57
1:B:294:GLY:HA3	1:B:297:TYR:CE2	2.39	0.57
2:J:73:ASP:HB3	2:J:78:LEU:HB2	1.86	0.57
3:L:120:VAL:O	3:L:209:LYS:NZ	2.30	0.57



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:L:33:ASN:OD1	3:L:68:LYS:NZ	2.34	0.57
3:K:37:TRP:HB2	3:K:50:LEU:HB2	1.87	0.57
1:A:297:TYR:HB3	1:A:330:CYS:HA	1.87	0.57
3:K:113:GLN:CB	3:K:114:PRO:HD3	2.23	0.57
1:A:238[A]:HIS:CG	1:A:239:ALA:N	2.73	0.57
2:F:35:MET:HB3	2:F:50:TYR:HD1	1.70	0.57
2:J:91:THR:HG23	2:J:114:THR:HA	1.86	0.57
3:L:143:ASP:OD1	3:L:172:GLN:NE2	2.31	0.57
1:B:334:VAL:HG22	1:B:378:VAL:HG22	1.87	0.57
2:N:5:VAL:HG22	2:N:23:ALA:HB3	1.86	0.56
1:B:358:THR:OG1	1:B:361:ASP:OD1	2.23	0.56
1:A:69:LYS:NZ	1:A:84:GLU:OE2	2.36	0.56
2:J:52:SER:O	2:J:72:ARG:NH1	2.38	0.56
2:Q:142:LEU:HD13	2:Q:215:VAL:HG11	1.88	0.56
1:A:298:LYS:O	1:A:330:CYS:HB2	2.06	0.56
3:L:153:TRP:HE1	3:L:181:SER:HG	1.52	0.56
3:L:199:GLN:HB3	3:L:208:GLU:HG3	1.86	0.56
1:E:252:GLY:O	1:E:256:THR:HG23	2.06	0.56
1:B:265:THR:HG22	1:B:266:LYS:H	1.70	0.56
2:C:36:TRP:HD1	2:C:70:ILE:HD12	1.70	0.56
1:E:202:SER:HB2	1:E:264:VAL:HB	1.88	0.56
1:B:39:PRO:HD2	1:B:290:LEU:HB3	1.87	0.56
1:B:328:ALA:CB	1:B:329:PRO:CD	2.65	0.56
1:I:95:THR:HG22	1:I:96:TYR:H	1.70	0.56
3:R:18:ILE:HD12	3:R:19:THR:H	1.71	0.56
3:G:49:ILE:HA	3:G:60:VAL:HG21	1.87	0.55
1:P:132:GLN:HE21	1:P:190:PHE:HB3	1.70	0.55
1:A:183:GLN:HG2	1:A:184:VAL:O	2.06	0.55
2:J:128:LEU:HB3	3:K:123:PHE:CE2	2.41	0.55
1:I:265:THR:HG22	1:I:266:LYS:H	1.71	0.55
3:L:150:THR:HB	3:L:201:THR:HB	1.89	0.55
2:J:73:ASP:N	2:J:78:LEU:O	2.36	0.55
2:J:185:VAL:HG11	3:K:140:LEU:HD13	1.87	0.55
2:J:192:SER:OG	2:J:198:TYR:OH	2.22	0.55
1:E:125:MET:SD	1:E:196:ALA:HB1	2.47	0.55
3:D:120:VAL:O	3:D:209:LYS:NZ	2.40	0.55
3:D:154:LYS:HE2	3:D:199:GLN:HE22	1.72	0.55
1:I:339:ASP:OD1	1:I:341:THR:N	2.36	0.55
1:B:238[A]:HIS:CG	1:B:239:ALA:N	2.73	0.54
2:C:63:SER:O	2:C:67:ARG:NH1	2.40	0.54
3:K:6:GLN:HB2	3:K:21:SER:O	2.08	0.54



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Atom-1	Atom-2	distance (Å)	overlap (Å)
3:O:18:ILE:HG22	3:O:77:ILE:CG1	2.37	0.54
1:P:215:LEU:HD21	1:P:250:GLN:HG3	1.89	0.54
1:E:61:TYR:CZ	1:E:123:LYS:HB3	2.42	0.54
2:J:52:SER:HB3	2:J:57:GLN:HB2	1.89	0.54
1:B:62:SER:HB3	1:B:123:LYS:HB2	1.88	0.54
1:B:99:ARG:NH1	1:B:103:ASN:O	2.36	0.54
3:D:56:ARG:HH11	3:D:62:ASN:HA	1.71	0.54
1:I:4:ILE:HD13	1:I:319:VAL:HG11	1.88	0.54
1:M:307:VAL:HG23	1:M:323:LYS:HB2	1.89	0.54
3:R:2:ALA:HB3	3:R:101:VAL:HG11	1.89	0.54
3:K:2:ALA:HB1	3:K:101:VAL:HG11	1.89	0.54
1:P:132:GLN:NE2	1:P:190:PHE:HB3	2.22	0.54
2:C:11:LEU:HD12	2:C:11:LEU:C	2.28	0.54
1:M:219:SER:O	1:M:221:SER:N	2.37	0.54
2:J:175:GLN:NE2	2:J:179:LEU:O	2.41	0.54
1:M:329:PRO:HD3	1:M:357:SER:O	2.08	0.54
2:N:52:SER:HB2	2:N:57:GLN:HB2	1.90	0.54
1:P:310:PRO:HD2	1:P:387:TYR:CD2	2.43	0.54
3:R:41:HIS:CD2	3:R:86:ALA:HB2	2.43	0.54
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.90	0.54
1:P:309:ASN:HB3	1:P:387:TYR:HE2	1.73	0.54
2:F:172:ALA:HB2	2:F:182:LEU:HD23	1.90	0.53
3:L:33:ASN:HA	3:L:68:LYS:NZ	2.24	0.53
1:A:80:ALA:O	1:A:94:ARG:NH2	2.36	0.53
3:L:30:GLU:OE2	3:D:28:ASN:ND2	2.42	0.53
1:M:175:TYR:CZ	1:M:293:LYS:HB3	2.43	0.53
2:H:86:LEU:HB3	2:H:115:VAL:HG21	1.90	0.53
3:K:81:GLN:O	3:K:110:VAL:HG21	2.09	0.53
1:M:379:GLY:HA3	1:M:384:ARG:HA	1.89	0.53
2:N:68:PHE:HD1	2:N:83:MET:HA	1.74	0.53
3:O:53:VAL:HG11	3:O:68:LYS:CG	2.38	0.53
2:Q:4:LEU:HD11	2:Q:98:THR:HG23	1.89	0.53
3:R:2:ALA:CB	3:R:101:VAL:HG11	2.38	0.53
3:R:27:SER:O	3:R:28:ASN:HB2	2.07	0.53
1:A:215:LEU:HD21	1:A:250:GLN:HG3	1.91	0.53
3:G:199:GLN:HB3	3:G:208:GLU:HG2	1.91	0.53
2:C:203:ASN:HD21	2:C:205:LYS:NZ	2.06	0.53
2:J:11:LEU:HD21	2:J:150:PHE:HZ	1.74	0.53
2:N:64:VAL:HB	2:N:68:PHE:CD2	2.43	0.53
1:A:202:SER:HB2	1:A:264:VAL:O	2.09	0.53
2:Q:200:CYS:O	2:Q:212:ASP:HA	2.09	0.53



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:308:LYS:HB2	1:A:321:GLN:HB2	1.92	0.52
1:I:238:HIS:CG	1:I:239:ALA:N	2.77	0.52
2:J:170:PHE:CE2	3:K:180:SER:HB3	2.40	0.52
2:N:36:TRP:CE2	2:N:81:LEU:HB2	2.43	0.52
3:O:20:ILE:HD11	3:O:108:LEU:HD13	1.84	0.52
1:P:15:VAL:HG22	1:P:17:GLY:H	1.75	0.52
1:I:3:CYS:HB3	1:I:9:ARG:NE	2.24	0.52
1:P:189:ASP:HB2	1:P:262:MET:HE1	1.91	0.52
2:Q:169:THR:HG23	2:Q:184:SER:HB2	1.91	0.52
2:C:123:PRO:HB3	2:C:149:TYR:HB3	1.91	0.52
1:A:65:LEU:HD11	1:A:232:VAL:HG22	1.90	0.52
2:H:170:PHE:HD2	3:L:180:SER:HB3	1.74	0.52
2:F:130:PRO:HB3	2:F:142:LEU:CD1	2.39	0.52
1:E:8:ASP:HB3	1:E:29:LYS:HG2	1.91	0.52
2:C:11:LEU:HA	2:C:114:THR:O	2.10	0.52
1:I:298:LYS:NZ	1:I:328:ALA:O	2.42	0.52
1:M:354:PRO:O	1:M:355:ILE:HD13	2.10	0.52
3:D:167:THR:HG23	3:D:180:SER:O	2.10	0.52
3:G:63:ARG:HH22	3:G:84:ASP:CG	2.14	0.51
1:B:70:ILE:HD11	1:B:242:ILE:HB	1.92	0.51
1:A:309:ASN:HB3	1:A:387:TYR:HE2	1.75	0.51
2:H:4:LEU:HD11	2:H:98:THR:HG23	1.92	0.51
2:N:47:TRP:HZ2	3:O:98:ILE:O	1.93	0.51
2:J:143:GLY:HA3	2:J:185:VAL:HG12	1.91	0.51
2:C:125:VAL:HG21	2:C:202:VAL:HG21	1.92	0.51
1:M:1:ALA:HB3	1:M:140:ARG:HB3	1.92	0.51
1:P:64:VAL:HG23	1:P:122:ALA:HB2	1.92	0.51
1:B:171:GLU:HA	1:B:177:LYS:HA	1.92	0.51
2:C:121:LYS:HD2	2:C:148:ASP:O	2.09	0.51
1:I:349:LEU:HD12	1:I:367:VAL:HG13	1.91	0.51
2:J:127:PRO:HD3	2:J:213:LYS:HE3	1.92	0.51
1:P:99:ARG:HA	1:P:103:ASN:HD21	1.75	0.51
3:K:4:LEU:HD22	3:K:29:ILE:HD11	1.92	0.51
2:N:4:LEU:HD11	2:N:98:THR:HG23	1.93	0.51
1:A:55:GLU:OE2	1:A:220:GLY:HA3	2.10	0.51
2:H:52:SER:HB3	2:H:57:GLN:HB2	1.93	0.51
1:B:294:GLY:HA3	1:B:297:TYR:CD2	2.45	0.51
3:L:34:LEU:HD11	3:L:93:TYR:HB3	1.93	0.51
3:D:2:ALA:HB3	3:D:101:VAL:HG21	1.93	0.51
1:P:132:GLN:HE21	1:P:186:THR:HB	1.75	0.51
1:E:64:VAL:HG13	1:E:122:ALA:HB2	1.92	0.50



	AL O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:80:ALA:O	1:E:94:ARG:NH2	2.45	0.50
3:K:127:SER:HA	3:K:130:LEU:HD12	1.91	0.50
2:F:50:TYR:HB3	2:F:59:TYR:HB2	1.92	0.50
1:B:26:GLU:HB2	1:B:29:LYS:HD2	1.93	0.50
1:B:237:PRO:HG3	1:B:242:ILE:HD11	1.93	0.50
2:N:45:LEU:HD12	3:O:89:PHE:CD2	2.47	0.50
2:J:214:ARG:HD3	2:J:216:GLU:HG3	1.94	0.50
1:M:12:ILE:O	1:M:33:VAL:HA	2.11	0.50
1:M:252:GLY:O	1:M:256:THR:HG23	2.12	0.50
1:A:310:PRO:HD2	1:A:387:TYR:CD2	2.46	0.50
1:B:192:ASN:C	1:B:207:ARG:HG3	2.32	0.50
3:L:146:PRO:HD2	3:L:203:GLU:OE2	2.12	0.50
1:B:188:VAL:HG12	1:B:188:VAL:O	2.12	0.50
2:J:68:PHE:CD1	2:J:83:MET:HA	2.47	0.50
2:J:73:ASP:OD2	2:J:76:LYS:HB2	2.12	0.50
2:Q:130:PRO:HG3	2:Q:142:LEU:HB3	1.94	0.50
1:A:95:THR:HG22	1:A:96:TYR:H	1.77	0.50
1:B:179:THR:HB	1:B:286:LYS:HB3	1.94	0.50
2:C:130:PRO:HB3	2:C:142:LEU:HD23	1.94	0.50
3:D:130:LEU:H	3:D:130:LEU:HD12	1.77	0.50
1:A:152:TRP:O	1:A:156:ILE:HG13	2.12	0.49
1:I:292:LEU:HD21	1:I:352:VAL:HG12	1.94	0.49
1:P:93:LYS:HD2	1:P:234:PHE:HB2	1.94	0.49
1:B:185:GLN:O	1:B:187:ALA:N	2.44	0.49
3:L:37:TRP:HB2	3:L:50:LEU:HB2	1.94	0.49
3:G:109:THR:HG21	3:G:146:PRO:HB3	1.94	0.49
1:I:304:MET:HG2	1:I:324:VAL:HG22	1.93	0.49
3:K:193:HIS:HB2	3:K:196:TYR:HE1	1.76	0.49
1:P:265:THR:OG1	1:P:277:HIS:NE2	2.34	0.49
1:A:335:ILE:HG13	1:A:377:ILE:HB	1.95	0.49
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.93	0.49
1:I:149:GLN:HG2	1:I:152:TRP:CE3	2.47	0.49
3:K:51:TYR:O	3:K:55:GLU:HB2	2.11	0.49
2:N:40:ALA:HB3	2:N:43:LYS:HB2	1.95	0.49
3:K:29:ILE:HG22	3:K:68:LYS:CE	2.40	0.49
2:N:202:VAL:HB	2:N:211:VAL:HG22	1.93	0.49
1:E:338:ASP:OD1	1:E:338:ASP:N	2.46	0.49
2:C:87:ARG:O	2:C:115:VAL:HG21	2.13	0.49
3:D:150:THR:HB	3:D:201:THR:HB	1.94	0.49
1:M:178:ALA:HB2	1:M:290:LEU:HD13	1.95	0.49
3:R:113:GLN:HB3	3:R:114:PRO:HD3	1.95	0.49



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:85:GLU:OE1	3:D:109:THR:HA	2.13	0.49
1:I:252:GLY:O	1:I:256:THR:HG23	2.12	0.49
1:P:328:ALA:HB1	1:P:329:PRO:HD2	1.53	0.49
1:E:66:THR:HG22	1:E:118:LYS:H	1.76	0.49
2:F:35:MET:SD	2:F:37:ILE:HD11	2.53	0.49
2:C:91:THR:HG23	2:C:114:THR:HA	1.94	0.49
2:N:36:TRP:NE1	2:N:81:LEU:HB2	2.28	0.49
1:A:12:ILE:HD12	1:A:31:VAL:HG11	1.95	0.48
1:B:45:LEU:HD11	1:B:48:VAL:HG23	1.94	0.48
1:B:149:GLN:HE21	1:B:150:GLU:HG3	1.78	0.48
3:K:27:SER:O	3:K:29:ILE:N	2.33	0.48
3:O:18:ILE:HG22	3:O:77:ILE:HG13	1.94	0.48
1:P:334:VAL:O	1:P:349:LEU:HD11	2.13	0.48
1:B:99:ARG:HA	1:B:103:ASN:HD21	1.78	0.48
1:I:137:TYR:CZ	1:I:161:PHE:HB2	2.48	0.48
2:N:89:GLU:OE1	2:N:89:GLU:N	2.36	0.48
3:O:165:GLU:OE1	3:O:165:GLU:HA	2.13	0.48
2:Q:83:MET:HB3	2:Q:86:LEU:HD21	1.94	0.48
2:Q:50:TYR:HB3	2:Q:59:TYR:HB2	1.95	0.48
1:E:34:MET:CE	1:E:350:VAL:HA	2.44	0.48
1:E:46:GLN:HG3	1:E:140:ARG:NH2	2.28	0.48
1:P:217:TRP:CZ2	1:P:226:ARG:HD3	2.47	0.48
1:A:26:GLU:HB2	1:A:29:LYS:HD2	1.95	0.48
1:A:194:TYR:CE2	1:A:207:ARG:HG3	2.49	0.48
1:E:125:MET:HE2	1:E:254:LEU:HD13	1.95	0.48
3:D:128:GLU:N	3:D:128:GLU:OE1	2.46	0.48
1:I:374:SER:OG	1:I:375:TYR:N	2.46	0.48
2:Q:204:HIS:CD2	2:Q:206:PRO:HD2	2.47	0.48
3:D:95:ASP:OD1	3:D:98:ILE:HG12	2.13	0.48
1:M:97:SER:OG	1:M:239:ALA:HA	2.13	0.48
1:M:218:GLN:HB2	1:M:225:TRP:CZ3	2.48	0.48
3:G:172:GLN:HG3	3:G:174:ASN:OD1	2.14	0.48
2:C:18:LEU:HD12	2:C:19:ARG:H	1.79	0.48
2:C:159:ASN:OD1	2:C:198:TYR:HA	2.13	0.48
3:0:124:PRO:HA	3:O:137:LEU:HD23	1.94	0.48
1:A:76:SER:HB3	1:P:130:VAL:O	2.13	0.48
2:C:141:ALA:HB2	2:C:187:THR:HG22	1.96	0.48
2:C:107:TRP:CE3	3:D:46:PRO:HG2	2.49	0.48
2:J:185:VAL:HG11	3:K:140:LEU:CD1	2.43	0.48
3:L:82:ALA:HA	3:L:110:VAL:HG21	1.96	0.47
1:M:266:LYS:NZ	1:M:266:LYS:HB3	2.29	0.47



	lo us puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:4:LEU:HD11	2:J:98:THR:HG23	1.96	0.47
1:B:38:LYS:HD2	1:B:290:LEU:HB2	1.96	0.47
1:M:157:LYS:HE2	1:M:172:PHE:CD1	2.49	0.47
2:Q:89:GLU:N	2:Q:89:GLU:OE1	2.46	0.47
1:E:150:GLU:OE1	1:E:150:GLU:N	2.41	0.47
3:D:56:ARG:NH1	3:D:62:ASN:HA	2.30	0.47
3:K:157:SER:O	3:K:157:SER:OG	2.22	0.47
1:A:190:PHE:HE2	1:A:276:LEU:HD13	1.79	0.47
1:E:129:GLU:HG2	1:B:76:SER:HA	1.96	0.47
1:E:335:ILE:HG13	1:E:377:ILE:HB	1.97	0.47
1:M:293:LYS:HG2	1:M:294:GLY:N	2.29	0.47
3:L:139:CYS:HB2	3:L:153:TRP:CH2	2.49	0.47
1:B:96:TYR:HB3	1:B:110:LYS:HB3	1.97	0.47
1:B:218:GLN:HG2	1:B:219:SER:H	1.80	0.47
2:C:142:LEU:HD11	2:C:198:TYR:CE2	2.38	0.47
1:M:240:ALA:HB1	2:N:56:SER:HB2	1.96	0.47
1:E:38:LYS:NZ	1:E:290:LEU:O	2.28	0.47
1:I:339:ASP:OD1	1:I:340:LEU:N	2.48	0.47
3:O:143:ASP:OD1	3:O:172:GLN:NE2	2.37	0.47
1:A:38:LYS:NZ	1:A:290:LEU:O	2.41	0.47
1:A:238[A]:HIS:CG	1:A:239:ALA:H	2.33	0.47
1:A:328:ALA:CB	1:A:329:PRO:CD	2.70	0.47
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.97	0.47
3:L:34:LEU:CD1	3:L:93:TYR:HB3	2.44	0.47
3:L:85:GLU:HG3	3:L:108:LEU:O	2.15	0.47
1:B:94:ARG:HG3	1:B:94:ARG:HH11	1.80	0.47
3:K:121:THR:HG22	3:K:123:PHE:CE1	2.49	0.47
1:E:145:VAL:HG12	1:E:146:GLY:H	1.80	0.47
1:B:66:THR:HG22	1:B:118:LYS:H	1.78	0.47
1:B:161:PHE:N	1:B:161:PHE:HD1	2.13	0.47
1:I:96:TYR:HB3	1:I:110:LYS:HB3	1.96	0.47
3:K:185:LEU:HD11	3:K:196:TYR:CE2	2.50	0.47
1:M:61:TYR:CZ	1:M:123:LYS:HB3	2.50	0.47
2:Q:125:VAL:HB	2:Q:211:VAL:HG11	1.96	0.47
1:I:65:LEU:HD11	1:I:232:VAL:HG22	1.97	0.46
1:I:313:THR:HG22	1:I:319:VAL:HG22	1.96	0.46
3:O:99:PHE:HD1	3:O:99:PHE:HA	1.62	0.46
1:P:180:LEU:HD23	1:P:180:LEU:HA	1.78	0.46
3:R:98:ILE:HD12	3:R:98:ILE:HA	1.71	0.46
3:G:18:ILE:HG23	3:G:80:LEU:HD21	1.98	0.46
2:C:125:VAL:CG2	2:C:202:VAL:HG21	2.46	0.46



	h h	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:J:68:PHE:CE1	2:J:83:MET:HG2	2.49	0.46	
1:P:50:ILE:CD1	1:P:130:VAL:HG13	2.44	0.46	
3:L:51:TYR:O	3:L:55:GLU:HB2	2.16	0.46	
1:I:128:PHE:HB2	1:I:195:ILE:HB	1.97	0.46	
2:J:20:LEU:HD22	2:J:111:THR:HG21	1.98	0.46	
1:P:129:GLU:HG3	1:P:194:TYR:HE1	1.80	0.46	
1:P:307:VAL:CG2	1:P:323:LYS:HB2	2.46	0.46	
2:J:67:ARG:NH1	2:J:90:ASP:OD2	2.35	0.46	
3:0:71:ASN:OD1	3:R:25:THR:HG23	2.16	0.46	
1:P:252:GLY:O	1:P:256:THR:HG23	2.15	0.46	
3:R:109:THR:HG21	3:R:146:PRO:HB3	1.96	0.46	
1:A:44:SER:OG	1:A:140:ARG:HB2	2.16	0.46	
2:H:170:PHE:CD2	3:L:180:SER:HB3	2.50	0.46	
2:H:204:HIS:HB3	2:H:209:THR:HB	1.98	0.46	
2:C:37:ILE:HD12	2:C:107:TRP:CH2	2.50	0.46	
1:P:129:GLU:HG3	1:P:194:TYR:CE1	2.50	0.46	
1:B:60:CYS:HB2	1:B:225:TRP:CZ3	2.51	0.46	
2:C:60:TYR:CE1	2:C:70:ILE:HG22	2.51	0.46	
2:H:203:ASN:OD1	2:H:205:LYS:NZ	2.49	0.46	
1:E:82:LEU:HB3	1:E:84:GLU:HG2	1.97	0.46	
1:B:67:HIS:HB3	3:D:96:THR:HG23	1.97	0.46	
3:O:137:LEU:HD12	3:O:183:LEU:HD23	1.98	0.46	
3:R:32:TYR:HB3	3:R:34:LEU:CD2	2.45	0.46	
1:E:3:CYS:HB3	1:E:9:ARG:HG3	1.97	0.46	
2:J:67:ARG:HD2	2:J:85:SER:O	2.16	0.46	
1:M:3:CYS:HB3	1:M:9:ARG:NE	2.30	0.46	
3:R:116:ALA:HB3	3:R:145:TYR:N	2.30	0.46	
1:A:226:ARG:HH22	1:P:85:GLU:HG2	1.81	0.46	
3:L:63:ARG:NH1	3:L:84:ASP:OD2	2.49	0.46	
1:E:132:GLN:NE2	1:E:190:PHE:O	2.49	0.46	
1:B:161:PHE:N	1:B:161:PHE:CD1	2.84	0.46	
3:L:171:LYS:HD3	3:L:177:TYR:CE1	2.51	0.46	
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.98	0.46	
1:B:65:LEU:HD21	1:B:232:VAL:HG21	1.98	0.46	
1:B:265:THR:HG1	1:B:277:HIS:CD2	2.33	0.46	
2:C:91:THR:OG1	2:C:115:VAL:HG22	2.16	0.46	
3:K:25:THR:O	3:K:71:ASN:ND2	2.49	0.46	
3:K:133:ASN:HA	3:K:187:PRO:HG3	1.98	0.46	
1:P:206:ASP:OD1	1:P:207:ARG:N	2.49	0.46	
3:O:13:SER:HB2	3:O:16:GLN:NE2	2.30	0.45	
3:R:28:ASN:HA	3:R:94:ALA:HA	1.98	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:R:38:TYR:HB2	3:R:89:PHE:HB2	1.98	0.45	
2:F:52:SER:HB3	2:F:57:GLN:HB2	1.97	0.45	
2:F:83:MET:HE1	2:F:94:TYR:CZ	2.51	0.45	
1:B:146:GLY:HA2	1:B:364:LEU:O	2.16	0.45	
1:A:129:GLU:HG3	1:A:194:TYR:CE1	2.51	0.45	
1:B:379:GLY:HA3	1:B:384:ARG:HA	1.98	0.45	
1:I:89:ASP:HA	1:I:228:MET:HE1	1.98	0.45	
3:K:144:PHE:CE1	3:K:178:ALA:HA	2.51	0.45	
1:P:46:GLN:HG3	1:P:140:ARG:HE	1.81	0.45	
2:Q:100:THR:O	2:Q:103:ARG:HG2	2.16	0.45	
3:L:25:THR:O	3:L:27:SER:N	2.48	0.45	
3:D:34:LEU:H	3:D:34:LEU:HG	1.64	0.45	
2:J:209:THR:HG22	2:J:211:VAL:HG23	1.97	0.45	
3:K:32:TYR:HB3	3:K:34:LEU:HD23	1.97	0.45	
1:M:320:MET:HG2	1:M:365:ILE:HB	1.96	0.45	
1:M:374:SER:OG	1:M:375:TYR:N	2.49	0.45	
2:N:109:GLN:NE2	2:N:110:GLY:O	2.49	0.45	
1:P:329:PRO:O	1:P:329:PRO:HG2	2.17	0.45	
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.97	0.45	
2:C:204:HIS:CE1	2:C:206:PRO:HG2	2.51	0.45	
1:P:334:VAL:HG22	1:P:378:VAL:HG22	1.97	0.45	
3:R:53:VAL:CG1	3:R:68:LYS:HB2	2.46	0.45	
1:B:202:SER:HB2	1:B:264:VAL:O	2.17	0.45	
2:C:154:VAL:HG12	2:C:182:LEU:HD21	1.99	0.45	
1:M:334:VAL:HG22	1:M:378:VAL:HG13	1.98	0.45	
3:O:115:LYS:HD2	3:O:203:GLU:HG3	1.99	0.45	
2:H:143:GLY:HA3	2:H:184:SER:O	2.17	0.45	
3:K:113:GLN:OE1	3:K:114:PRO:HD2	2.16	0.45	
1:M:233:GLU:HG3	1:M:247:LEU:HD21	1.98	0.45	
2:N:47:TRP:CZ2	3:O:99:PHE:HB2	2.51	0.45	
2:N:130:PRO:HB3	2:N:142:LEU:HB3	1.98	0.45	
3:O:29:ILE:HD13	3:O:73:ALA:HB2	1.98	0.45	
1:E:4:ILE:HD13	1:E:319:VAL:HG11	1.98	0.45	
1:I:50:ILE:HD11	1:I:276:LEU:HD21	1.99	0.45	
2:J:50:TYR:HB3	2:J:59:TYR:HB2	1.98	0.45	
1:M:179:THR:HB	1:M:286:LYS:HB3	1.97	0.45	
1:E:304:MET:O	1:E:385:LEU:HD21	2.17	0.45	
1:M:132:GLN:CD	1:M:132:GLN:H	2.20	0.45	
2:N:6:GLU:HG2	2:N:96:CYS:SG	2.57	0.45	
2:Q:29:PHE:O	2:Q:72:ARG:NH2	2.49	0.45	
1:E:150:GLU:H	1:E:150:GLU:CD	2.20	0.45	



	lo uo puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:202:VAL:HG22	2:C:211:VAL:HB	1.99	0.45	
3:D:95:ASP:OD1	3:D:95:ASP:N	2.49	0.45	
1:E:349:LEU:HD12	1:E:367:VAL:HG12	2.00	0.44	
1:B:297:TYR:HE1	1:B:329:PRO:HB3	1.81	0.44	
1:I:225:TRP:HB2	1:I:228:MET:HE3	2.00	0.44	
2:N:154:VAL:HG12	2:N:204:HIS:CD2	2.49	0.44	
1:A:26:GLU:HG2	1:A:280:HIS:HB3	2.00	0.44	
1:E:308:LYS:HG3	1:E:321:GLN:HB2	2.00	0.44	
1:M:50:ILE:HD11	1:M:190:PHE:CE2	2.49	0.44	
2:H:203:ASN:OD1	2:H:210:LYS:HG2	2.17	0.44	
3:L:130:LEU:HD22	3:L:187:PRO:HB3	1.99	0.44	
1:I:318:VAL:HG12	1:I:369:PRO:HD3	1.98	0.44	
1:I:177:LYS:NZ	1:I:179:THR:OG1	2.49	0.44	
1:P:237:PRO:HB3	1:P:242:ILE:HG12	1.99	0.44	
1:B:302:ASP:N	1:B:302:ASP:OD1	2.50	0.44	
3:D:63:ARG:HB3	3:D:78:SER:O	2.17	0.44	
1:M:1:ALA:HA	1:M:2:HIS:HA	1.62	0.44	
1:B:69:LYS:NZ	1:B:84:GLU:OE2	2.40	0.44	
1:P:206:ASP:HB3	1:P:209:TRP:HB3	1.99	0.44	
1:E:307:VAL:CG2	1:E:323:LYS:HB2	2.48	0.44	
1:E:371:PHE:CD1	1:E:371:PHE:N	2.86	0.44	
2:F:12:VAL:O	2:F:115:VAL:HA	2.18	0.44	
2:J:38:ARG:HD3	2:J:94:TYR:CE2	2.53	0.44	
2:N:168:HIS:HB3	2:N:170:PHE:HE1	1.83	0.44	
1:B:157:LYS:HG2	1:B:172:PHE:CE1	2.53	0.44	
3:R:115:LYS:HG2	3:R:116:ALA:N	2.32	0.44	
3:O:17:SER:HA	3:0:77:ILE:O	2.18	0.43	
3:O:93:TYR:HA	3:O:100:TRP:HA	2.00	0.43	
1:E:9:ARG:HB3	1:E:315:HIS:CD2	2.52	0.43	
1:E:186:THR:HA	1:E:189:ASP:OD2	2.19	0.43	
2:F:68:PHE:CZ	2:F:83:MET:HE2	2.54	0.43	
1:B:121:CYS:SG	1:B:124:SER:HB3	2.58	0.43	
2:C:199:ILE:HG22	2:C:213:LYS:C	2.39	0.43	
3:D:63:ARG:HH22	3:D:84:ASP:CG	2.22	0.43	
1:M:135:ILE:HD13	1:M:186:THR:HG21	1.99	0.43	
2:H:20:LEU:HB2	2:H:81:LEU:HB3	2.00	0.43	
2:H:205:LYS:HA	2:H:205:LYS:HD3	1.71	0.43	
2:C:135:THR:HG22	2:C:135:THR:O	2.16	0.43	
3:K:171:LYS:HD2	3:K:175:ASN:HA	2.00	0.43	
2:N:68:PHE:CE1	2:N:83:MET:HE3	2.53	0.43	
1:P:34:MET:HG2	1:P:40:SER:OG	2.18	0.43	



	louis page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:R:6:GLN:HG3	3:R:106:THR:OG1	2.18	0.43	
1:A:130:VAL:O	1:P:76:SER:HB3	2.18	0.43	
3:L:6:GLN:HG3	3:L:106:THR:OG1	2.18	0.43	
2:N:47:TRP:CE2	3:O:99:PHE:HB2	2.54	0.43	
1:A:266:LYS:HB3	1:A:266:LYS:HE2	1.69	0.43	
2:H:35:MET:SD	2:H:104:ILE:HG12	2.58	0.43	
1:E:56:ALA:O	1:B:79:GLU:HG3	2.19	0.43	
1:B:185:GLN:C	1:B:187:ALA:H	2.21	0.43	
1:B:377:ILE:HG23	1:B:384:ARG:HD3	1.99	0.43	
2:C:169:THR:HG22	2:C:184:SER:HB2	2.01	0.43	
1:I:171:GLU:HA	1:I:177:LYS:HA	2.00	0.43	
2:J:168:HIS:CD2	3:K:178:ALA:HB3	2.54	0.43	
1:A:349:LEU:HD12	1:A:367:VAL:HG22	2.01	0.43	
2:H:29:PHE:O	2:H:72:ARG:NH2	2.52	0.43	
1:B:252:GLY:O	1:B:256:THR:HG23	2.18	0.43	
1:I:218:GLN:HB2	1:I:225:TRP:CZ3	2.54	0.43	
3:K:34:LEU:HA	3:K:52:GLU:HA	2.01	0.43	
2:N:45:LEU:HD12	3:O:89:PHE:CE2	2.54	0.43	
1:P:221:SER:O	1:P:223:GLY:N	2.43	0.43	
3:L:53:VAL:CG1	3:L:68:LYS:HB2	2.48	0.43	
1:E:65:LEU:HD21	1:E:232:VAL:HG13	2.01	0.43	
1:E:74:CYS:O	1:E:77:THR:HB	2.19	0.43	
3:G:160:VAL:HG11	3:G:183:LEU:HD11	1.99	0.43	
1:B:103:ASN:HD22	1:B:239:ALA:HB1	1.84	0.43	
3:D:6:GLN:HG3	3:D:106:THR:OG1	2.19	0.43	
3:D:139:CYS:C	3:D:140:LEU:HD23	2.39	0.43	
1:I:217:TRP:CZ2	1:I:226:ARG:HD3	2.53	0.43	
1:M:130:VAL:HG22	1:M:195:ILE:HG13	2.01	0.43	
1:E:267:ASP:O	1:E:269:ASN:N	2.52	0.43	
3:D:33:ASN:O	3:D:53:VAL:HG12	2.19	0.43	
1:M:38:LYS:HG3	1:M:290:LEU:O	2.19	0.43	
3:L:141:ILE:HG12	3:L:200:VAL:HG21	2.00	0.43	
1:E:237:PRO:HB3	1:E:242:ILE:HG12	2.01	0.43	
1:M:340:LEU:HD21	1:M:386:THR:HG21	2.01	0.43	
1:A:369:PRO:O	1:A:391:LYS:NZ	2.34	0.42	
3:L:18:ILE:HG12	3:L:19:THR:N	2.34	0.42	
2:H:127:PRO:O	3:L:126:SER:OG	2.36	0.42	
1:B:215:LEU:HD21	1:B:250:GLN:HG3	2.01	0.42	
3:K:99:PHE:O	3:K:100:TRP:CG	2.72	0.42	
1:M:336:VAL:HG21	1:M:367:VAL:HG11	2.01	0.42	
1:P:30:CYS:HB2	1:P:44:SER:HB3	2.01	0.42	



	to ac page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:P:84:GLU:OE1	1:P:84:GLU:N	2.48	0.42	
1:P:265:THR:HG22	1:P:266:LYS:H	1.84	0.42	
1:P:340:LEU:HD23	1:P:340:LEU:HA	1.79	0.42	
1:E:199:GLU:HG2	1:E:199:GLU:O	2.19	0.42	
2:C:142:LEU:HD21	2:C:198:TYR:OH	2.18	0.42	
3:D:137:LEU:HB2	3:D:183:LEU:HB3	2.01	0.42	
3:R:124:PRO:HA	3:R:137:LEU:HD13	2.02	0.42	
1:B:323:LYS:HE3	1:B:325:PRO:HD3	2.02	0.42	
1:M:304:MET:O	1:M:385:LEU:HD21	2.18	0.42	
2:N:36:TRP:CZ2	2:N:79:LEU:HD23	2.55	0.42	
2:Q:123:PRO:HD2	2:Q:209:THR:HG21	2.00	0.42	
3:L:193:HIS:HB2	3:L:196:TYR:HE1	1.84	0.42	
2:F:52:SER:O	2:F:72:ARG:NH1	2.53	0.42	
1:M:218:GLN:HB2	1:M:225:TRP:CE3	2.54	0.42	
2:Q:36:TRP:CG	2:Q:81:LEU:HD22	2.55	0.42	
1:B:190:PHE:C	1:B:192:ASN:H	2.23	0.42	
2:C:52:SER:HB3	2:C:57:GLN:HB2	2.00	0.42	
3:D:10:VAL:HG23	3:D:18:ILE:HD11	2.00	0.42	
1:I:238:HIS:CG	1:I:239:ALA:H	2.38	0.42	
1:M:195:ILE:HG21	1:M:274:TYR:CD2	2.54	0.42	
2:N:87:ARG:O	2:N:115:VAL:HG21	2.20	0.42	
2:N:134:SER:O	2:N:135:THR:OG1	2.31	0.42	
1:B:149:GLN:HA	1:B:152:TRP:CG	2.55	0.42	
1:B:334:VAL:HG21	1:B:365:ILE:HD13	2.02	0.42	
1:I:1:ALA:HA	1:I:2:HIS:HA	1.64	0.42	
2:J:68:PHE:HB3	2:J:81:LEU:HD11	2.02	0.42	
2:Q:123:PRO:HB3	2:Q:149:TYR:HB3	2.01	0.42	
1:A:310:PRO:HA	1:A:319:VAL:O	2.19	0.42	
1:E:183:GLN:NE2	1:E:185:GLN:OE1	2.53	0.42	
1:B:149:GLN:HA	1:B:152:TRP:CD2	2.54	0.42	
3:D:28:ASN:HD22	3:D:28:ASN:HA	1.69	0.42	
1:M:33:VAL:CG2	1:M:41:LEU:HB3	2.50	0.42	
1:M:236:PRO:HA	1:M:237:PRO:HD3	1.90	0.42	
1:P:95:THR:HG22	1:P:96:TYR:N	2.30	0.42	
1:E:159:LEU:HD12	1:E:180:LEU:HD12	2.01	0.42	
2:F:142:LEU:HD23	2:F:215:VAL:CG1	2.50	0.42	
2:J:128:LEU:HB3	3:K:123:PHE:CD2	2.55	0.42	
3:R:51:TYR:O	3:R:55:GLU:HB2	2.19	0.42	
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.48	0.41	
1:E:329:PRO:CD	1:E:357:SER:O	2.56	0.41	
1:M:39:PRO:HB2	1:M:143:LEU:HD22	2.02	0.41	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:Q:37:ILE:HD11	2:Q:104:ILE:HD13	2.02	0.41	
1:A:146:GLY:HA3	1:A:363:VAL:HG13	2.00	0.41	
2:C:4:LEU:HD11	2:C:98:THR:HG23	2.01	0.41	
1:B:194:TYR:CD2	1:B:207:ARG:HG2	2.55	0.41	
2:J:167:VAL:HG22	2:J:186:VAL:HB	2.02	0.41	
3:K:62:ASN:OD1	3:K:62:ASN:N	2.51	0.41	
3:K:171:LYS:HG3	3:K:172:GLN:N	2.36	0.41	
1:E:57:ARG:NH2	1:E:211:GLN:HG2	2.35	0.41	
1:E:264:VAL:HG22	1:E:276:LEU:HD13	2.03	0.41	
3:D:199:GLN:HB3	3:D:208:GLU:HG3	2.02	0.41	
1:I:299:MET:HE3	1:I:299:MET:HB3	1.90	0.41	
2:J:93:LEU:HD12	2:J:111:THR:C	2.40	0.41	
1:P:318:VAL:HG12	1:P:369:PRO:HD3	2.01	0.41	
2:Q:143:GLY:HA2	2:Q:185:VAL:HA	2.01	0.41	
2:H:35:MET:HB3	2:H:50:TYR:HD1	1.86	0.41	
3:G:200:VAL:O	3:G:206:THR:HA	2.20	0.41	
1:B:236:PRO:HA	1:B:237:PRO:HD3	1.88	0.41	
2:C:214:ARG:HH11	2:C:214:ARG:CG	2.33	0.41	
2:N:63:SER:O	2:N:67:ARG:NH2	2.54	0.41	
2:N:125:VAL:HA	2:N:145:LEU:O	2.20	0.41	
1:P:224:ILE:HD12	1:P:226:ARG:HG3	2.01	0.41	
1:E:293:LYS:O	1:E:355:ILE:HD11	2.20	0.41	
1:B:348:ILE:HB	1:B:368:ASN:HB3	2.03	0.41	
3:O:41:HIS:CD2	3:O:86:ALA:HB2	2.56	0.41	
3:O:167:THR:HG21	3:O:180:SER:H	1.85	0.41	
1:P:150:GLU:H	1:P:150:GLU:HG3	1.57	0.41	
1:A:9:ARG:HD2	1:A:315:HIS:ND1	2.35	0.41	
1:A:190:PHE:CE2	1:A:276:LEU:HD13	2.56	0.41	
1:B:1:ALA:HA	1:B:2:HIS:HA	1.67	0.41	
3:O:61:SER:OG	3:O:63:ARG:HG3	2.20	0.41	
1:P:262:MET:SD	1:P:278:GLY:HA3	2.61	0.41	
1:A:263:ARG:NH1	1:B:235:GLU:OE2	2.54	0.41	
3:L:12:GLY:O	3:L:110:VAL:HA	2.21	0.41	
1:B:99:ARG:HD3	1:B:239:ALA:O	2.21	0.41	
3:D:80:LEU:HD12	3:D:80:LEU:HA	1.82	0.41	
1:I:66:THR:HG23	3:K:93:TYR:CZ	2.56	0.41	
1:M:298:LYS:NZ	1:M:328:ALA:O	2.54	0.41	
2:Q:67:ARG:HB3	2:Q:84:ASN:O	2.21	0.41	
3:R:120:VAL:O	3:R:209:LYS:HE3	2.20	0.41	
2:H:67:ARG:HB3	2:H:84:ASN:O	2.21	0.41	
1:I:143:LEU:HD21	1:I:290:LEU:HD21	2.02	0.41	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:I:236:PRO:HA	1:I:237:PRO:HD3	1.92	0.41	
3:K:99:PHE:HB3	3:K:100:TRP:CE3	2.55	0.41	
1:M:80:ALA:HB3	1:M:114:VAL:HG23	2.02	0.41	
1:B:298:LYS:O	1:B:330:CYS:HB2	2.22	0.40	
1:P:1:ALA:HA	1:P:2:HIS:HA	1.73	0.40	
3:R:175:ASN:OD1	3:R:175:ASN:N	2.53	0.40	
1:A:57:ARG:HB2	1:A:127:LEU:HD12	2.04	0.40	
1:E:325:PRO:O	1:E:359:ASN:HB3	2.21	0.40	
1:B:39:PRO:HD3	1:B:292:LEU:HD13	2.03	0.40	
1:B:194:TYR:CE2	1:B:207:ARG:HG2	2.56	0.40	
2:C:158:TRP:HA	2:C:199:ILE:O	2.21	0.40	
2:C:174:LEU:HD13	2:C:180:TYR:CE1	2.55	0.40	
3:D:144:PHE:CE1	3:D:147:GLY:HA2	2.56	0.40	
2:J:63:SER:OG	2:J:64:VAL:HG13	2.21	0.40	
1:M:258:LEU:HD23	1:M:258:LEU:HA	1.87	0.40	
2:N:86:LEU:HD23	2:N:86:LEU:HA	1.84	0.40	
2:N:107:TRP:CE3	3:O:46:PRO:HG2	2.56	0.40	
3:R:153:TRP:CE3	3:R:183:LEU:HD12	2.56	0.40	
2:H:205:LYS:N	2:H:205:LYS:HE2	2.37	0.40	
3:L:144:PHE:CE2	3:L:147:GLY:HA2	2.57	0.40	
3:D:93:TYR:HA	3:D:100:TRP:HA	2.03	0.40	
2:N:104:ILE:HD12	3:O:102:PHE:HZ	1.86	0.40	
1:A:62:SER:HB3	1:A:123:LYS:HB2	2.03	0.40	
3:L:70:GLY:HA3	3:D:27:SER:HA	2.03	0.40	
3:G:172:GLN:H	3:G:172:GLN:HG2	1.66	0.40	
1:B:8:ASP:OD2	1:B:29:LYS:HE2	2.22	0.40	
2:C:34:MET:HB3	2:C:79:LEU:HD22	2.03	0.40	
1:I:8:ASP:HB3	1:I:29:LYS:HG2	2.04	0.40	
2:N:12:VAL:O	2:N:115:VAL:HA	2.22	0.40	
2:N:216:GLU:HG2	2:N:217:PRO:HD2	2.04	0.40	
2:Q:173:VAL:HB	3:R:167:THR:HG22	2.02	0.40	
1:A:149:GLN:NE2	1:B:101:TRP:O	2.55	0.40	
1:A:226:ARG:NH2	1:P:85:GLU:HG2	2.37	0.40	
1:B:67:HIS:CE1	2:C:102:TRP:CD1	3.09	0.40	
3:R:6:GLN:HB2	3:R:21:SER:O	2.22	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	391/398~(98%)	369~(94%)	19 (5%)	3~(1%)	19	49
1	В	385/398~(97%)	363~(94%)	19 (5%)	3(1%)	19	49
1	Е	390/398~(98%)	367~(94%)	19 (5%)	4 (1%)	15	44
1	Ι	384/398~(96%)	363~(94%)	19 (5%)	2~(0%)	29	61
1	М	384/398~(96%)	365~(95%)	17 (4%)	2(0%)	29	61
1	Р	384/398~(96%)	364~(95%)	19 (5%)	1 (0%)	41	72
2	С	214/217~(99%)	203~(95%)	10 (5%)	1 (0%)	29	61
2	F	214/217~(99%)	208~(97%)	6 (3%)	0	100	100
2	Н	214/217~(99%)	205~(96%)	9 (4%)	0	100	100
2	J	207/217~(95%)	197~(95%)	8 (4%)	2 (1%)	15	44
2	Ν	214/217~(99%)	202 (94%)	12 (6%)	0	100	100
2	Q	214/217~(99%)	205~(96%)	9 (4%)	0	100	100
3	D	211/217~(97%)	199 (94%)	9~(4%)	3~(1%)	11	34
3	G	214/217~(99%)	197~(92%)	15 (7%)	2(1%)	17	46
3	Κ	212/217~(98%)	194 (92%)	16 (8%)	2(1%)	17	46
3	L	212/217~(98%)	198~(93%)	10 (5%)	4 (2%)	8	26
3	Ο	215/217~(99%)	201 (94%)	8 (4%)	6(3%)	5	17
3	R	211/217~(97%)	196 (93%)	13 (6%)	2 (1%)	17	46
All	All	4870/4992 (98%)	4596 (94%)	237 (5%)	37 (1%)	19	49

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	329	PRO
3	L	26	GLY
1	Е	267	ASP
1	Ε	268	GLU



Mol	Chain	Res	Type
1	Е	329	PRO
1	В	329	PRO
2	С	160	SER
3	D	30	GLU
1	Ι	329	PRO
2	J	123	PRO
1	М	329	PRO
3	0	26	GLY
3	0	99	PHE
3	0	113	GLN
3	0	114	PRO
1	Р	328	ALA
1	А	268	GLU
3	L	27	SER
3	G	99	PHE
3	D	53	VAL
2	J	124	SER
3	R	27	SER
3	L	99	PHE
1	А	269	ASN
3	G	114	PRO
1	В	186	THR
3	K	113	GLN
1	М	328	ALA
1	Ι	328	ALA
3	L	53	VAL
3	0	53	VAL
1	Е	328	ALA
3	D	29	ILE
3	О	98	ILE
3	K	53	VAL
1	В	188	VAL
3	R	53	VAL

5.3.2 Protein sidechains (i)

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

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



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	327/330~(99%)	315~(96%)	12 (4%)	34	68
1	В	322/330~(98%)	306~(95%)	16 (5%)	24	56
1	Ε	324/330~(98%)	312~(96%)	12 (4%)	34	68
1	Ι	320/330~(97%)	311~(97%)	9~(3%)	43	77
1	М	319/330~(97%)	309~(97%)	10 (3%)	40	74
1	Р	319/330~(97%)	307~(96%)	12 (4%)	33	67
2	С	182/183~(100%)	173~(95%)	9~(5%)	25	57
2	F	182/183~(100%)	180 (99%)	2 (1%)	73	92
2	Н	182/183~(100%)	174 (96%)	8 (4%)	28	61
2	J	178/183~(97%)	168 (94%)	10 (6%)	21	51
2	Ν	182/183~(100%)	176 (97%)	6 (3%)	38	72
2	Q	182/183~(100%)	180 (99%)	2(1%)	73	92
3	D	179/183~(98%)	172~(96%)	7 (4%)	32	66
3	G	182/183~(100%)	173~(95%)	9~(5%)	25	57
3	К	180/183~(98%)	176~(98%)	4 (2%)	52	83
3	L	180/183~(98%)	174 (97%)	6 (3%)	38	72
3	Ο	183/183 (100%)	176 (96%)	7 (4%)	33	67
3	R	179/183~(98%)	171 (96%)	8 (4%)	27	60
All	All	$410\overline{2/4176}~(98\%)$	3953~(96%)	149 (4%)	35	69

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	10	ASP
1	А	120	THR
1	А	132	GLN
1	А	149	GLN
1	А	164	LEU
1	А	190	PHE
1	А	238[A]	HIS
1	А	238[B]	HIS
1	А	243	ARG
1	А	329	PRO
1	А	380	THR
1	А	387	TYR
2	Н	19	ARG
2	Н	43	LYS



Mol	Chain	Res	Type
2	Н	46	GLU
2	Н	49	SER
2	Н	85	SER
2	Н	89	GLU
2	Н	205	LYS
2	Н	213	LYS
3	L	17	SER
3	L	34	LEU
3	L	61	SER
3	L	109	THR
3	L	113	GLN
3	L	199	GLN
1	Е	8	ASP
1	Е	9	ARG
1	Е	15	VAL
1	Е	57	ARG
1	Е	89	ASP
1	Е	120	THR
1	Ε	140	ARG
1	Ε	153	ASN
1	Ε	263	ARG
1	Ε	265	THR
1	Ε	329	PRO
1	Ε	339	ASP
2	F	117	SER
2	F	165	SER
3	G	34	LEU
3	G	113	GLN
3	G	119	SER
3	G	133	ASN
3	G	142	SER
3	G	165	GLU
3	G	170	SER
3	G	181	SER
3	G	188	GLU
1	В	2	HIS
1	В	9	ARG
1	В	24	THR
1	В	161	PHE
1	В	171	GLU
1	В	189	ASP
1	В	243	ARG



Mol	Chain	Res	Type
1	В	263	ARG
1	В	299	MET
1	В	302	ASP
1	В	320	MET
1	В	329	PRO
1	В	339	ASP
1	В	380	THR
1	В	383	SER
1	В	384	ARG
2	С	43	LYS
2	С	78	LEU
2	С	109	GLN
2	С	116	SER
2	С	121	LYS
2	С	163	LEU
2	С	198	TYR
2	С	213	LYS
2	С	214	ARG
3	D	34	LEU
3	D	53	VAL
3	D	85	GLU
3	D	149	VAL
3	D	186	THR
3	D	191	LYS
3	D	205	SER
1	Ι	243	ARG
1	Ι	276	LEU
1	Ι	286	LYS
1	Ι	299	MET
1	Ι	340	LEU
1	Ι	355	ILE
1	Ι	363	VAL
1	Ι	374	SER
1	Ι	380	THR
2	J	63	SER
2	J	109	GLN
2	J	115	VAL
2	J	117	SER
2	J	174	LEU
2	J	175	GLN
2	J	179	LEU
2	J	192	SER



Mol	Chain	Res	Type
2	J	200	CYS
2	J	203	ASN
3	K	27	SER
3	K	34	LEU
3	K	140	LEU
3	Κ	157	SER
1	М	10	ASP
1	М	38	LYS
1	М	87	ASP
1	М	89	ASP
1	М	120	THR
1	М	132	GLN
1	М	148	LYS
1	М	190	PHE
1	М	199	GLU
1	М	295	THR
2	Ν	17	SER
2	Ν	38	ARG
2	Ν	79	LEU
2	Ν	85	SER
2	Ν	87	ARG
2	Ν	183	SER
3	0	27	SER
3	0	68	LYS
3	0	99	PHE
3	0	108	LEU
3	0	114	PRO
3	0	141	ILE
3	Ο	145	TYR
1	Р	120	THR
1	Р	177	LYS
1	Р	190	PHE
1	Р	199	GLU
1	P	$26\overline{2}$	MET
1	Р	265	THR
1	P	303	LYS
1	Р	320	MET
1	Р	331	LYS
1	P	380	THR
1	Р	382	ASP
1	Р	387	TYR
2	Q	147	LYS



Continued from previous page			
Mol	Chain	Res	Type
2	Q	205	LYS
3	R	17	SER
3	R	21	SER
3	R	34	LEU
3	R	74	SER
3	R	98	ILE
3	R	145	TYR
3	R	171	LYS
3	R	208	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	132	GLN
1	А	211	GLN
3	L	28	ASN
3	L	62	ASN
3	G	16	GLN
1	В	149	GLN
2	С	203	ASN
3	D	28	ASN
2	J	203	ASN
1	М	277	HIS
2	N	77	ASN
2	N	175	GLN
3	0	6	GLN
1	Р	132	GLN
1	Р	144	HIS
2	Q	109	GLN
3	R	41	HIS

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)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

