



Full wwPDB X-ray Structure Validation Report

Jun 12, 2014 – 11:40 PM EDT

PDB ID : 4D0M
Title : Phosphatidylinositol 4-kinase III beta in a complex with Rab11a-GTP-gamma-S and the Rab-binding domain of FIP3
Authors : Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.
Deposited on : 2014-04-27
Resolution : 6.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

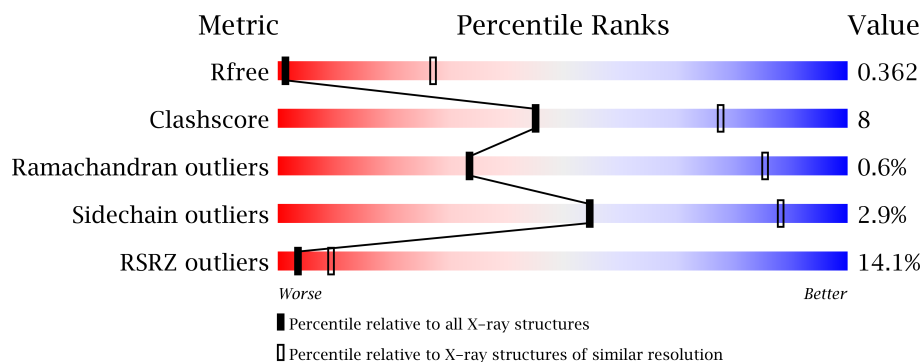
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 6.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1089 (8.20-3.50)
Clashscore	79885	1024 (8.20-3.52)
Ramachandran outliers	78287	1283 (8.50-3.50)
Sidechain outliers	78261	1259 (8.50-3.50)
RSRZ outliers	66119	1088 (8.20-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	566	
1	C	566	
1	G	566	
1	I	566	
1	M	566	
1	O	566	
1	Q	566	
1	S	566	
1	W	566	
1	Y	566	
1	c	566	
1	g	566	
2	B	219	
2	D	219	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	219	
2	J	219	
2	N	219	
2	P	219	
2	R	219	
2	T	219	
2	X	219	
2	Z	219	
2	d	219	
2	h	219	
3	E	48	
3	F	48	
3	K	48	
3	L	48	
3	U	48	
3	V	48	
3	a	48	
3	b	48	
3	e	48	
3	f	48	
3	i	48	
3	j	48	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 65970 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	C	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	G	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	I	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	M	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	O	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Q	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	S	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	W	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Y	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	c	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	g	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			

- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	D	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	J	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	N	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	P	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	R	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	T	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	X	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	Z	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	d	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	h	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
D	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
H	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
J	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
N	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
P	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
R	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
T	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
X	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
Z	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
d	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
h	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491

- Molecule 3 is a protein called RAB11 FAMILY-INTERACTING PROTEIN 3.

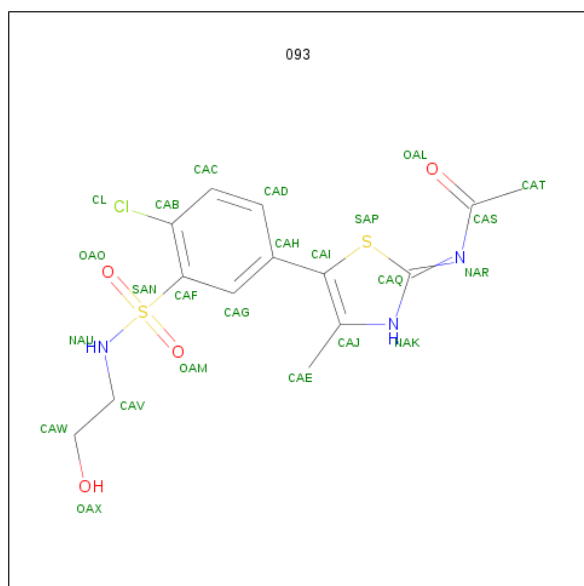
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			

Continued on next page...

Continued from previous page...

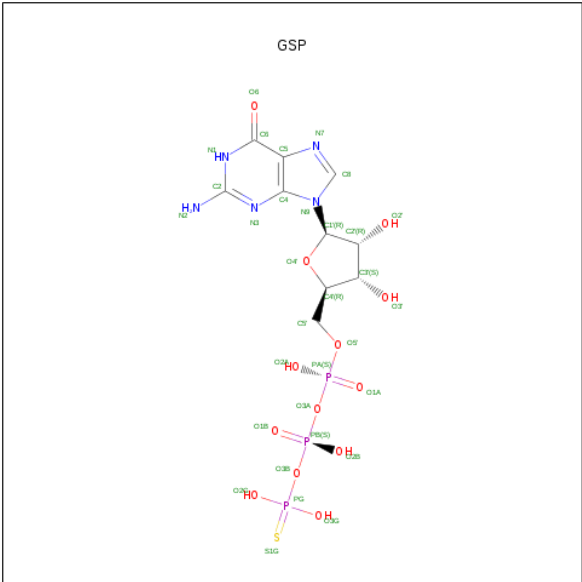
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	K	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	L	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	U	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	V	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	a	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	b	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	e	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	f	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	i	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	j	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			

- Molecule 4 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)-PHENYLTHIAZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	C	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	G	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	I	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	M	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	O	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	Q	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	S	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	W	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	Y	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	c	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	g	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	H	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	J	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	N	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	P	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	R	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	T	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	X	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	Z	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	d	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	h	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	H	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	h	1	Total	Mg	0	0
			1	1		
6	Z	1	Total	Mg	0	0
			1	1		
6	T	1	Total	Mg	0	0
			1	1		

Continued on next page...

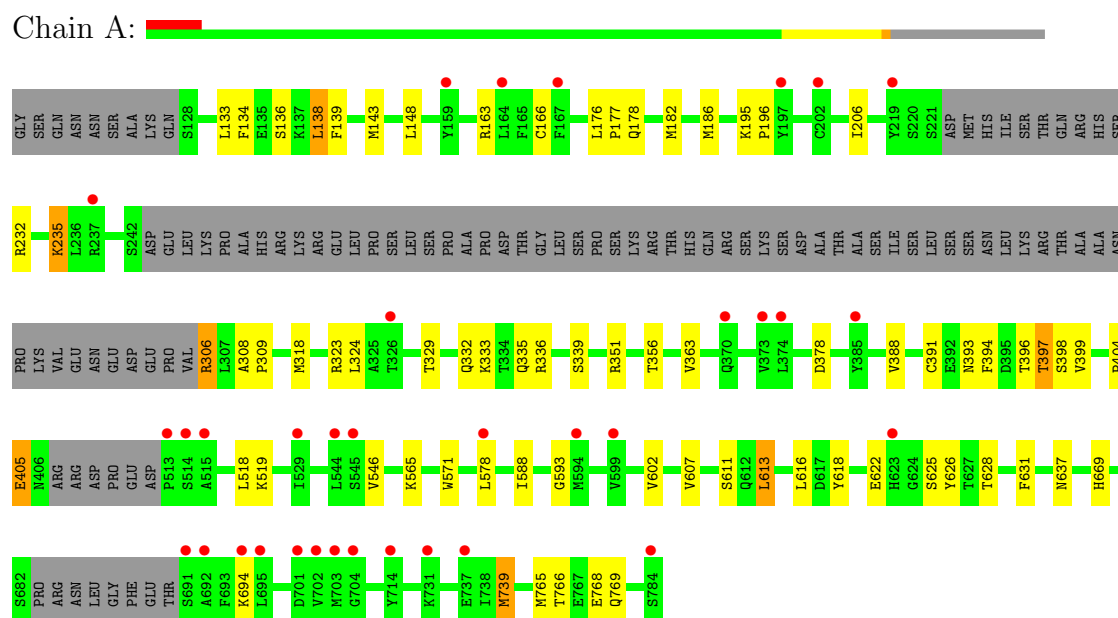
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	1	Total 1	Mg 1	0	0
6	X	1	Total 1	Mg 1	0	0
6	d	1	Total 1	Mg 1	0	0
6	R	1	Total 1	Mg 1	0	0

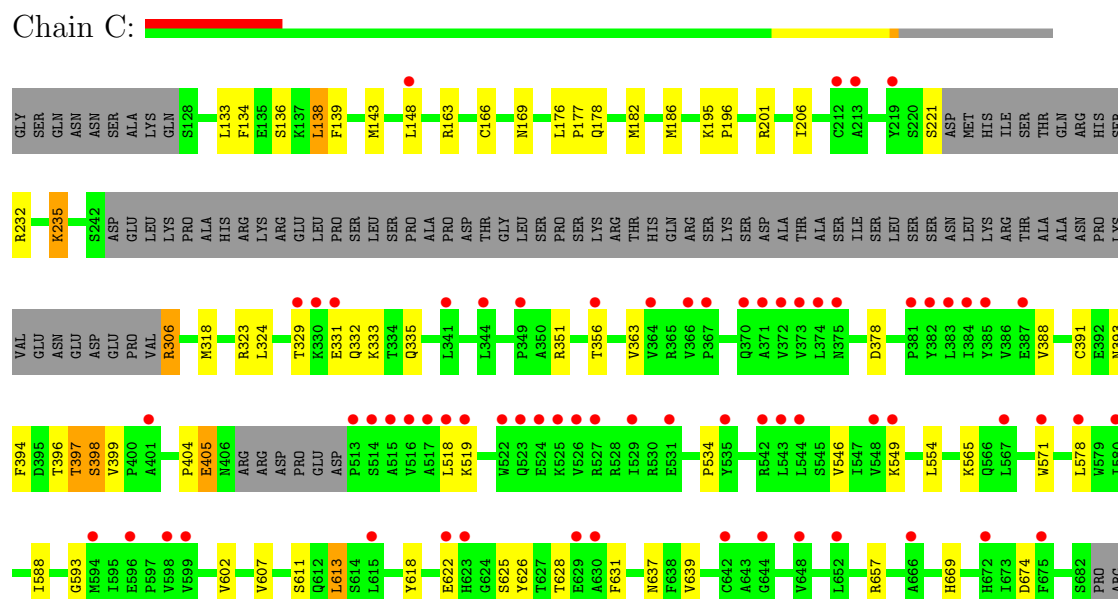
3 Residue-property plots

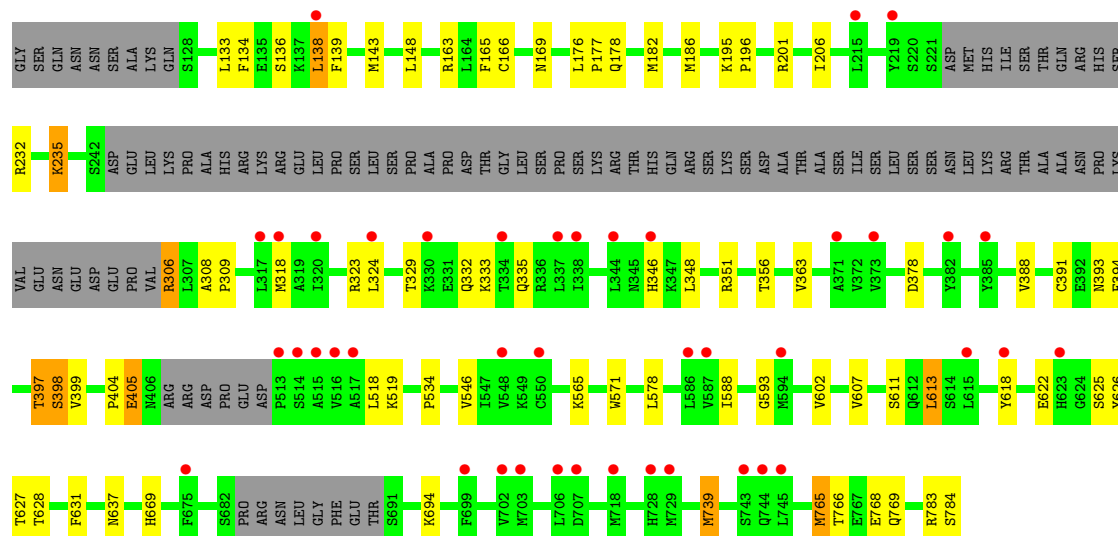
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PHOSPHATIDYLINOSITOL 4-KINASE BETA



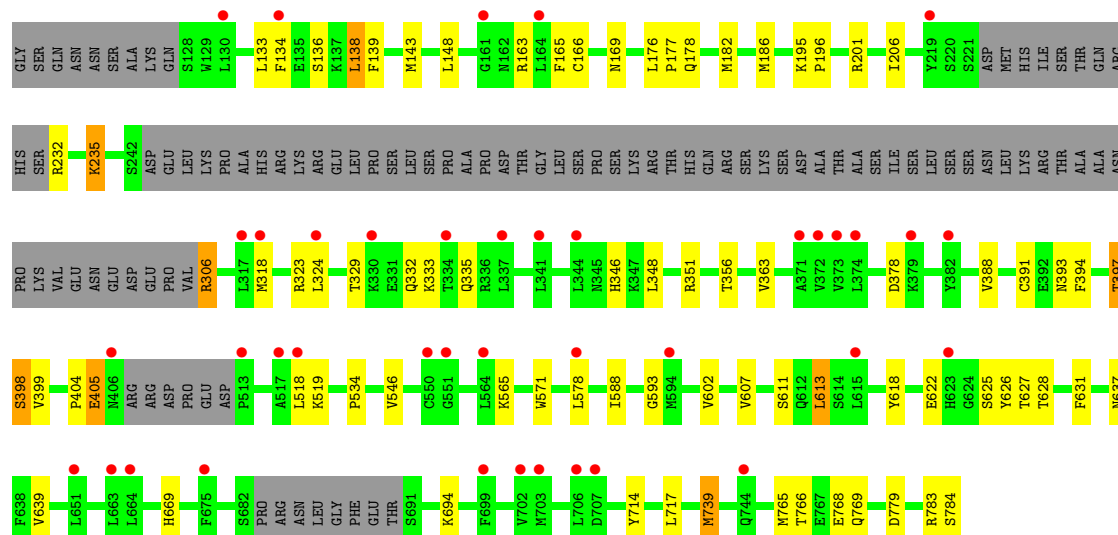
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA





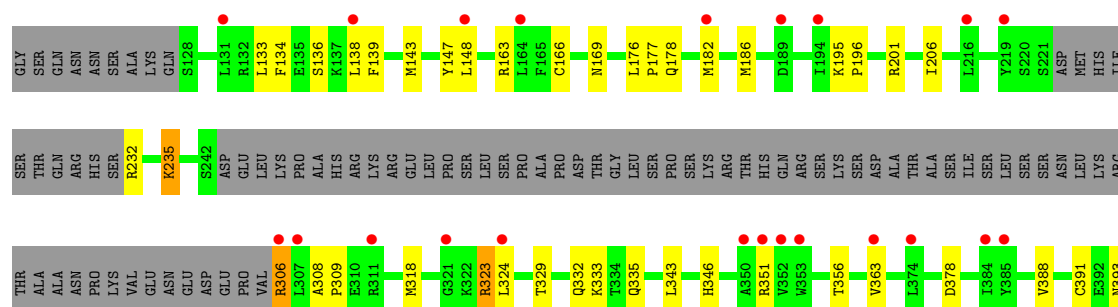
● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

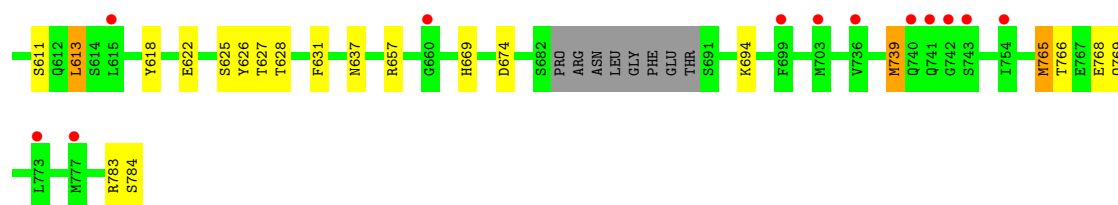
Chain O:



● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

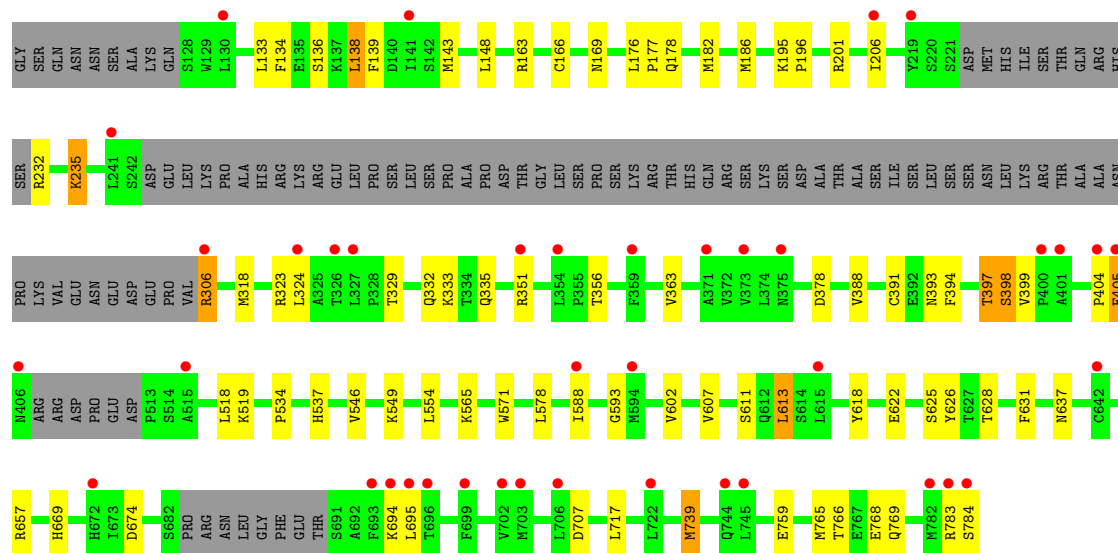
Chain Q:





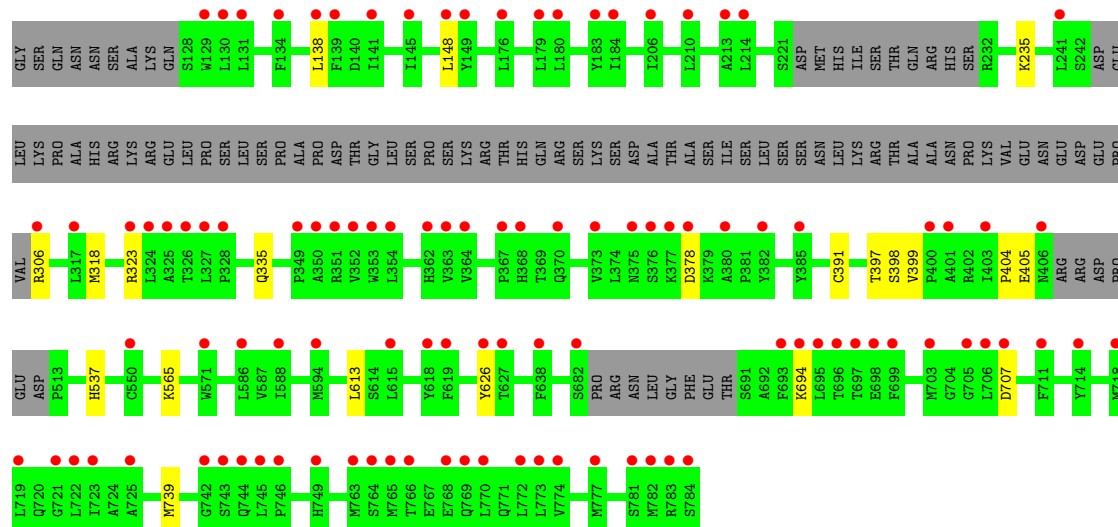
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain Y:



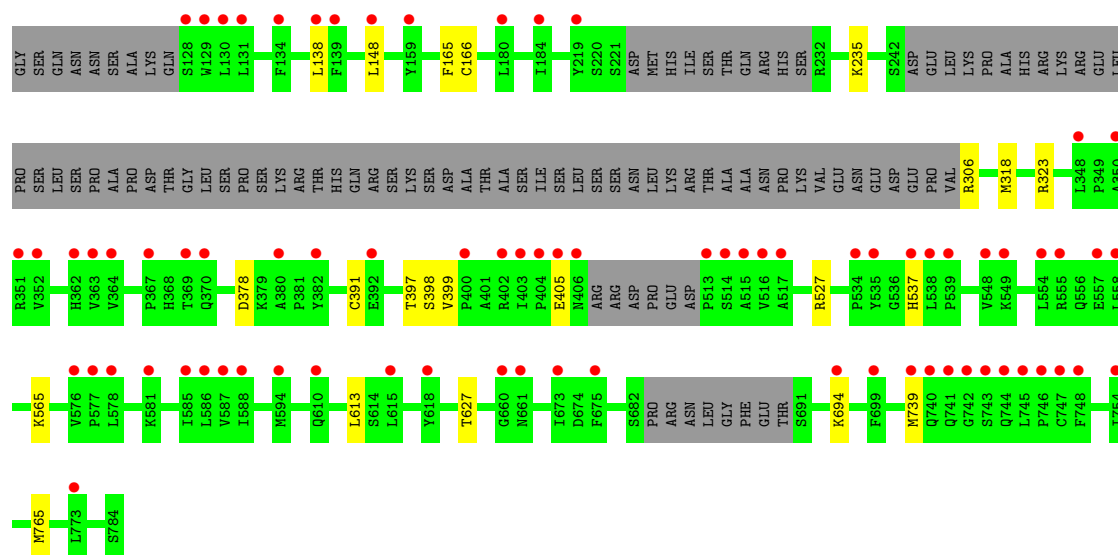
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain c:



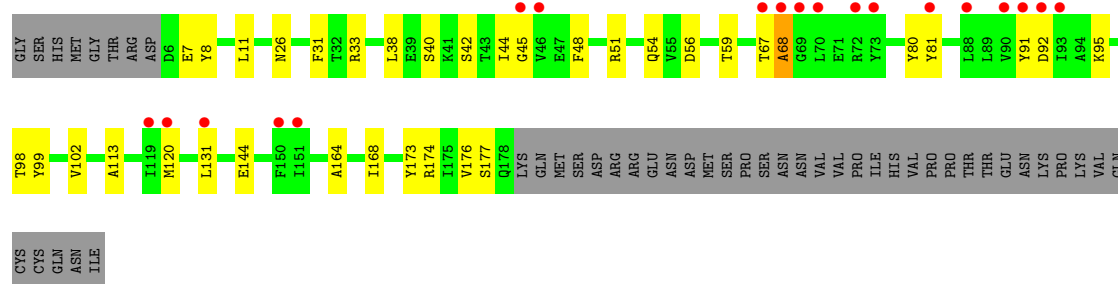
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain g:



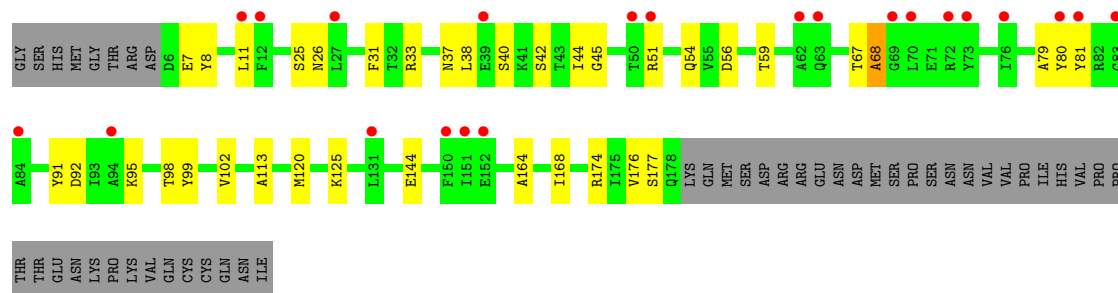
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain B:



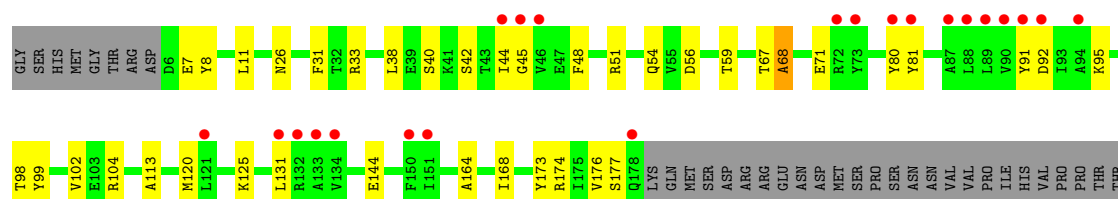
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain D:



• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain H:



GLU
ASN
LYS
PRO
LYS
VAL
GLN
CYS
CYS
ASN
ILE

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain J:

GLY SER HIS MET GLY THR ARG ASP D6 E7 Y8 L11 F12 F13 D19 N26 L27 F31 T32 R33 L38 E39 I44 G45 R51 Q54 V55 D56 G57 R58 T59 T67 A68 G69 L70 E71 R72 A79 Y80 Y81 Y91 D92 K95 T98 Y99

V102 A113 M120 L131 E144 Y150 A164 I168 Y174 Y178 LYS MET GLN SER ASP ARG ARG ASN ASP MET SER PRO THR VAL VAL ILE HIS VAL PRO THR THR GLN LYS PRO LYS VAL CYS CYS GLN ASN ILE

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain N:

GLY SER HIS MET GLY THR ARG ASP D6 E7 Y8 L11 F12 F13 K14 V14 V15 V16 V17 N26 F31 T32 R33 L38 E39 S40 K41 S42 T43 I44 G45 V46 E47 F48 A49 T50 R51 Q54 V55 D56 T59 A62 Q63 I64 T67 G69 G89 L70 E71 R72 R74

T77 Y81 G86 A87 L88 L89 V90 D92 K95 H96 L97 T98 Y99 V102 E103 R104 W105 L106 L109 R110 A113 I119 M120 L121 V122 L131 R140 E144 S149 F150 I151 A164 I168 R174 I175 V176 S177 Q178 LYS GLN MET SER ASP ARG ARG

GLU ASN MET PRO SER ASN VAL VAL PRO ILE HIS VAL PRO THR THR GLU ASN LYS PRO LYS VAL GLN CYS CYS GLN ILE

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain P:

GLY SER HIS MET GLY THR ARG ASP D6 E7 Y8 L11 F12 L16 I17 N26 F31 T32 R33 N37 L38 E39 S40 K41 S42 G45 V46 E47 F48 A49 T50 R51 Q54 V55 D56 T59 A62 Q63 T67 A68 G69 E71 R72 Y73 R74 A75 T77

Y81 R82 G83 A84 V85 G86 A87 L88 L89 V90 D92 T93 A94 K95 H96 L97 T98 Y99 V102 E103 R104 W105 L106 L109 L110 A113 I117 V118 I119 M120 L121 R129 H130 L131 E144 L148 S149 F150 A164 I168 R174 I175 V176 S177 Q178 LYS GLN MET SER ASP

ARG ARG ASN ASP MET SER PRO SER ASN VAL VAL PRO ILE HIS VAL PRO PRO THR THR GLU ASN LYS PRO LYS VAL GLN CYS CYS GLN ASN ILE

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

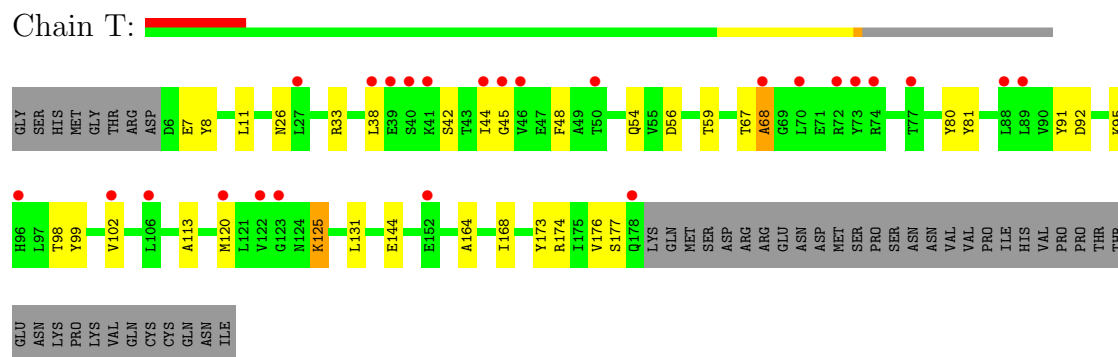
Chain R:

GLY SER HIS MET GLY THR ARG ASP D6 E7 Y8 L11 N26 L27 R33 L38 E39 S40 K41 I44 G45 V46 E47 F48 A49 T50 Q54 V55 D56 T59 T67 A68 R72 Y80 Y81 L89 Y91 D92 I93 A94 K95 H96 L97 T98 Y99 E100 E101 V102

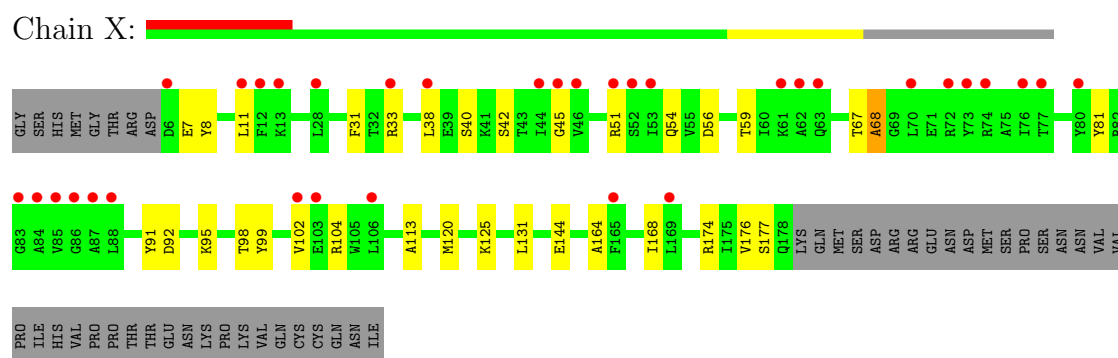
E103 R104 W105 L106 L109 R110 A113 I119 M120 L121 V122 G123 N124 K125 L131 E144 L148 S149 F150 I151 T152 T153 S154 A155 A164 F165 I168 R174 I175 V176 S177 Q178 LYS GLN MET SER ASP ARG GLU ASN ASP MET SER PRO SER ASN VAL VAL PRO

ILE HIS VAL PRO THR THR GLU ASN LYS LYS VAL GLN CYS CYS GLN ASN ILE

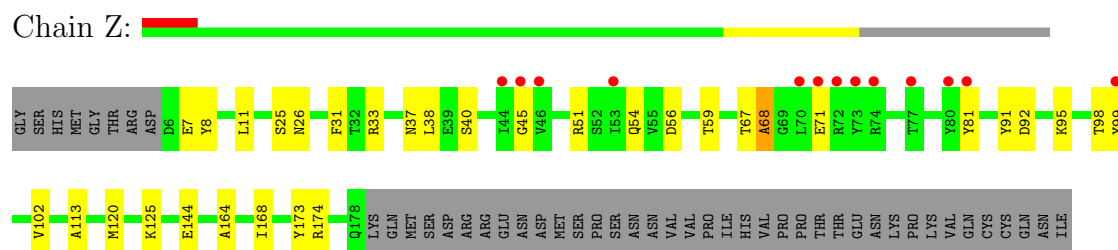
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



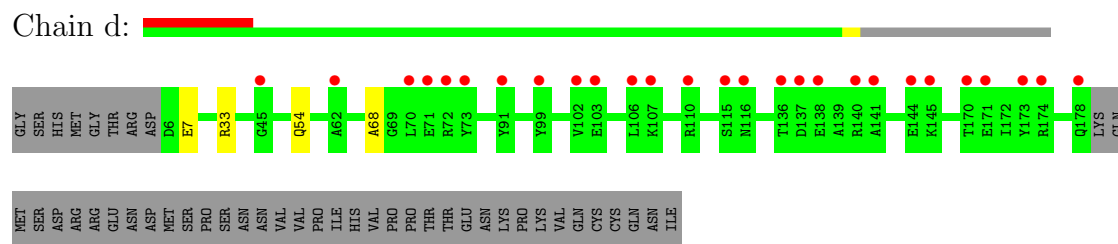
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



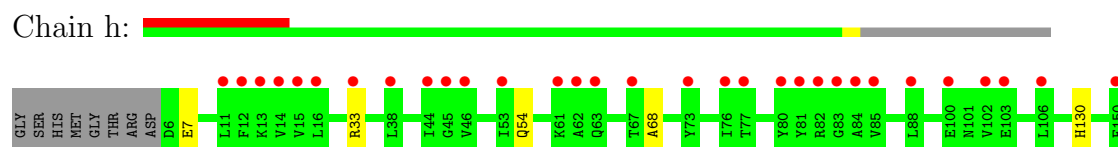
- Molecule 2: RAS-RELATED PROTEIN RAB-11A

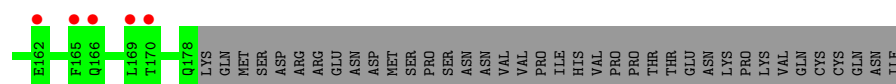


- Molecule 2: RAS-RELATED PROTEIN RAB-11A



- Molecule 2: RAS-RELATED PROTEIN RAB-11A





• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain E:



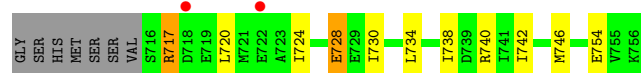
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain F:



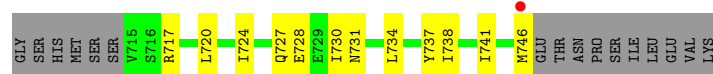
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain K:



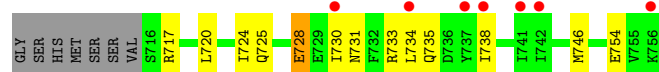
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain L:



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain U:



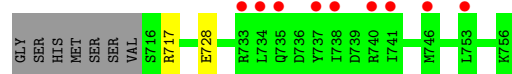
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain V:



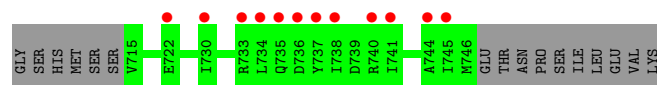
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain a:



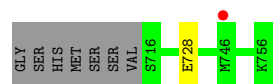
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain b: 



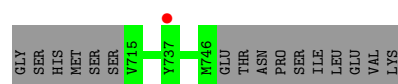
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain e: 



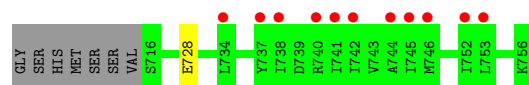
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain f: 



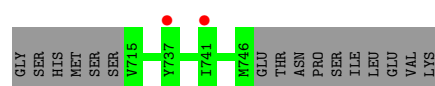
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain i: 



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain j: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	199.50Å 134.47Å 294.33Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	294.32 – 6.00 49.88 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (294.32-6.00) 93.0 (49.88-6.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.253 , 0.359 0.259 , 0.362	Depositor DCC
R_{free} test set	1925 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	248.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 258.8	EDS
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37330 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	65970	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, MG, 093

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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/3866	0.72	0/5219
1	C	0.56	0/3866	0.70	0/5219
1	G	0.59	0/3866	0.72	0/5219
1	I	0.56	0/3866	0.69	1/5219 (0.0%)
1	M	0.59	0/3866	0.71	1/5219 (0.0%)
1	O	0.59	0/3866	0.71	0/5219
1	Q	0.57	0/3866	0.70	0/5219
1	S	0.57	0/3866	0.70	0/5219
1	W	0.58	0/3866	0.70	1/5219 (0.0%)
1	Y	0.59	0/3866	0.70	0/5219
1	c	0.60	0/3866	0.71	0/5219
1	g	0.59	0/3866	0.70	2/5219 (0.0%)
2	B	0.64	0/1399	0.76	0/1892
2	D	0.61	0/1399	0.75	0/1892
2	H	0.63	0/1399	0.74	0/1892
2	J	0.63	0/1399	0.75	0/1892
2	N	0.58	0/1399	0.73	0/1892
2	P	0.59	0/1399	0.73	0/1892
2	R	0.59	0/1399	0.72	0/1892
2	T	0.58	0/1399	0.73	0/1892
2	X	0.58	0/1399	0.72	0/1892
2	Z	0.58	0/1399	0.73	0/1892
2	d	0.58	0/1399	0.73	0/1892
2	h	0.59	0/1399	0.72	0/1892
3	E	0.94	1/316 (0.3%)	0.98	1/429 (0.2%)
3	F	0.83	0/238	0.87	0/323
3	K	0.94	1/316 (0.3%)	0.97	1/429 (0.2%)
3	L	0.84	0/238	0.89	0/323
3	U	0.83	0/316	0.82	0/429
3	V	0.90	0/238	0.89	0/323
3	a	0.94	1/316 (0.3%)	0.96	1/429 (0.2%)
3	b	0.86	0/238	0.88	0/323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.85	0/316	0.86	0/429
3	f	0.88	0/238	0.89	0/323
3	i	0.85	0/316	0.81	0/429
3	j	0.88	0/238	0.87	0/323
All	All	0.60	3/66504 (0.0%)	0.72	8/89844 (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	A	0	1
1	C	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	O	0	1
1	Q	0	1
1	S	0	1
1	W	0	1
1	Y	0	1
1	c	0	1
1	g	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	717	ARG	CD-NE	5.41	1.55	1.46
3	E	717	ARG	CD-NE	5.12	1.55	1.46
3	K	717	ARG	CD-NE	5.07	1.55	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	a	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	E	717	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	g	527	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	I	132	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	M	765	MET	CG-SD-CE	5.09	108.35	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	765	MET	CG-SD-CE	5.05	108.28	100.20
1	W	765	MET	CG-SD-CE	5.03	108.25	100.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	398	SER	Peptide
1	G	398	SER	Peptide
1	I	398	SER	Peptide
1	M	398	SER	Peptide
1	O	398	SER	Peptide
1	Q	398	SER	Peptide
1	S	398	SER	Peptide
1	W	398	SER	Peptide
1	Y	398	SER	Peptide
1	c	398	SER	Peptide
1	g	398	SER	Peptide

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3788	0	3838	55	8
1	C	3788	0	3839	100	2
1	G	3788	0	3839	70	9
1	I	3788	0	3839	80	2
1	M	3788	0	3839	56	12
1	O	3788	0	3839	56	17
1	Q	3788	0	3839	62	4
1	S	3788	0	3839	65	12
1	W	3788	0	3838	56	4
1	Y	3788	0	3839	57	12
1	c	3788	0	3839	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	3788	0	3839	0	13
2	B	1377	0	1370	44	9
2	D	1377	0	1370	43	4
2	H	1377	0	1370	39	3
2	J	1377	0	1370	34	4
2	N	1377	0	1370	26	0
2	P	1377	0	1371	29	0
2	R	1377	0	1370	29	0
2	T	1377	0	1370	28	0
2	X	1377	0	1370	23	0
2	Z	1377	0	1371	24	0
2	d	1377	0	1370	0	0
2	h	1377	0	1370	0	1
3	E	314	0	298	89	0
3	F	237	0	222	78	0
3	K	314	0	298	52	0
3	L	237	0	222	35	0
3	U	314	0	298	23	0
3	V	237	0	222	47	0
3	a	314	0	298	0	0
3	b	237	0	222	0	0
3	e	314	0	298	0	0
3	f	237	0	222	0	0
3	i	314	0	298	0	0
3	j	237	0	222	0	0
4	A	24	0	16	0	0
4	C	24	0	16	0	0
4	G	24	0	16	0	0
4	I	24	0	16	0	0
4	M	24	0	16	0	0
4	O	24	0	16	0	0
4	Q	24	0	16	0	0
4	S	24	0	16	0	0
4	W	24	0	16	0	0
4	Y	24	0	16	0	0
4	c	24	0	16	0	0
4	g	24	0	16	0	0
5	B	32	0	12	6	0
5	D	32	0	12	11	0
5	H	32	0	12	7	0
5	J	32	0	12	4	0
5	N	32	0	12	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	32	0	12	7	0
5	R	32	0	12	5	0
5	T	32	0	12	5	0
5	X	32	0	12	6	0
5	Z	32	0	12	6	0
5	d	32	0	12	0	0
5	h	32	0	12	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	N	1	0	0	0	0
6	P	1	0	0	0	0
6	R	1	0	0	0	0
6	T	1	0	0	0	0
6	X	1	0	0	0	0
6	Z	1	0	0	1	0
6	d	1	0	0	0	0
6	h	1	0	0	0	0
All	All	65970	0	65964	993	61

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (993) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:44:ILE:HD11	3:K:734:LEU:CD2	1.30	1.59
2:J:44:ILE:CD1	3:K:734:LEU:HD22	1.30	1.59
2:D:44:ILE:HD11	3:E:734:LEU:CD2	1.41	1.50
1:C:138:LEU:HG	1:S:769:GLN:CG	1.41	1.48
2:D:44:ILE:CD1	3:E:734:LEU:HD22	1.44	1.47
1:C:138:LEU:CG	1:S:769:GLN:HG2	1.45	1.42
1:I:138:LEU:HG	1:Q:769:GLN:CG	1.52	1.38
1:I:138:LEU:CG	1:Q:769:GLN:HG2	1.53	1.34
1:G:138:LEU:HD21	1:M:765:MET:CE	1.59	1.30
1:A:138:LEU:HD21	1:O:765:MET:CE	1.63	1.27
3:F:728:GLU:CD	3:K:717:ARG:HD3	120.84	1.22
1:A:138:LEU:HD21	1:O:765:MET:HE3	1.23	1.18
2:B:80:TYR:OH	3:E:746:MET:CG	1.94	1.15
2:B:80:TYR:OH	3:E:746:MET:HG2	1.45	1.14
1:G:138:LEU:HD21	1:M:765:MET:HE2	1.23	1.13
2:H:80:TYR:OH	3:K:746:MET:HG2	1.48	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:731:ASN:HD21	3:F:731:ASN:CG	4.33	1.09
1:C:138:LEU:HD21	1:S:769:GLN:HB3	1.29	1.09
3:F:728:GLU:CD	3:K:717:ARG:CD	121.14	1.06
2:D:56:ASP:OD2	2:D:174:ARG:NH1	1.90	1.05
2:X:56:ASP:OD2	2:X:174:ARG:NH1	1.89	1.04
2:R:56:ASP:OD2	2:R:174:ARG:NH1	1.90	1.04
3:U:738:ILE:HD13	3:V:738:ILE:HD13	1.40	1.04
3:E:717:ARG:CG	3:V:728:GLU:OE2	2.06	1.04
2:H:56:ASP:OD2	2:H:174:ARG:NH1	1.91	1.04
1:I:138:LEU:HD21	1:Q:769:GLN:HB3	1.34	1.04
2:T:56:ASP:OD2	2:T:174:ARG:NH1	1.90	1.04
2:J:56:ASP:OD2	2:J:174:ARG:NH1	1.90	1.04
2:N:56:ASP:OD2	2:N:174:ARG:NH1	1.90	1.03
2:P:56:ASP:OD2	2:P:174:ARG:NH1	1.90	1.03
3:F:728:GLU:OE1	3:K:717:ARG:CD	121.62	1.03
1:G:769:GLN:HG2	1:Y:138:LEU:HG	182.13	1.02
3:E:738:ILE:HG21	3:F:738:ILE:HD11	3.82	1.02
2:Z:56:ASP:OD2	2:Z:174:ARG:NH1	1.90	1.02
3:K:738:ILE:HD13	3:L:738:ILE:CD1	1.90	1.01
3:E:717:ARG:HD3	3:V:728:GLU:CD	1.80	1.01
1:C:765:MET:HE3	1:W:138:LEU:HD21	140.06	1.01
2:B:56:ASP:OD2	2:B:174:ARG:NH1	1.92	1.01
1:C:138:LEU:HD21	1:W:765:MET:CE	142.94	1.01
2:J:44:ILE:HD11	3:K:734:LEU:HD21	1.43	1.00
2:J:44:ILE:HD13	3:K:734:LEU:HD22	1.43	0.99
2:H:48:PHE:HD2	3:K:754:GLU:HA	1.26	0.99
1:C:138:LEU:CG	1:S:769:GLN:CG	2.20	0.99
3:F:728:GLU:OE2	3:K:717:ARG:CG	119.50	0.98
3:F:728:GLU:OE2	3:K:717:ARG:HD3	119.80	0.97
2:D:44:ILE:HD11	3:E:734:LEU:HD21	1.46	0.97
2:J:79:ALA:CB	3:L:746:MET:CE	2.43	0.97
2:B:48:PHE:HD2	3:E:754:GLU:HA	1.29	0.96
3:E:731:ASN:ND2	3:F:731:ASN:CG	4.24	0.96
2:H:80:TYR:OH	3:K:746:MET:CG	2.13	0.95
1:G:138:LEU:CD2	1:M:765:MET:HE2	1.98	0.94
2:D:38:LEU:O	5:D:2000:GSP:O3'	2.20	0.93
1:A:138:LEU:CD2	1:O:765:MET:HE3	1.98	0.93
2:J:79:ALA:CB	3:L:746:MET:HE1	1.99	0.93
3:F:728:GLU:OE2	3:K:717:ARG:CD	120.10	0.93
3:U:738:ILE:HG21	3:V:738:ILE:HD11	1.51	0.92
2:J:79:ALA:HB3	3:L:746:MET:HE1	1.50	0.92
1:C:221:SER:O	2:Z:71:GLU:OE2	125.74	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:738:ILE:HD13	3:F:738:ILE:HD13	2.19	0.92
3:E:717:ARG:CD	3:V:728:GLU:CD	2.37	0.92
2:D:79:ALA:CB	3:F:746:MET:CE	2.48	0.91
1:C:138:LEU:HD23	1:S:769:GLN:CD	1.92	0.91
1:C:332:GLN:HE22	1:I:331:GLU:HG3	1.35	0.91
3:E:717:ARG:CD	3:V:724:ILE:HG22	2.01	0.90
1:G:138:LEU:HD21	1:M:765:MET:HE3	1.52	0.89
2:T:44:ILE:HD11	3:V:734:LEU:CD2	2.01	0.89
1:C:138:LEU:HD21	1:S:765:MET:HG2	1.55	0.89
3:E:738:ILE:HD13	3:F:738:ILE:HG12	1.54	0.88
1:G:765:MET:HG2	1:Y:138:LEU:HD21	179.51	0.88
2:B:48:PHE:CD2	3:E:754:GLU:HA	2.08	0.87
1:G:147:TYR:OH	1:Y:759:GLU:OE2	164.25	0.87
2:H:48:PHE:CD2	3:K:754:GLU:HA	2.09	0.87
3:E:717:ARG:HG3	3:V:728:GLU:CD	1.95	0.87
3:F:734:LEU:CD2	2:R:44:ILE:HD11	120.85	0.86
2:D:79:ALA:CB	3:F:746:MET:HE3	2.04	0.86
3:E:717:ARG:HG3	3:V:728:GLU:OE2	1.72	0.86
3:E:717:ARG:CD	3:V:728:GLU:OE1	2.24	0.86
1:C:138:LEU:CD2	1:S:769:GLN:HB3	2.06	0.86
1:G:138:LEU:CD2	1:M:765:MET:CE	2.49	0.85
1:G:769:GLN:CG	1:Y:138:LEU:HG	182.34	0.85
1:A:138:LEU:CD2	1:O:765:MET:CE	2.51	0.85
1:A:339:SER:OG	1:Y:537:HIS:HB2	1.75	0.85
3:F:734:LEU:HD21	2:R:44:ILE:HD11	120.57	0.84
1:C:138:LEU:CD2	1:S:769:GLN:CG	2.54	0.84
1:I:138:LEU:CG	1:Q:769:GLN:CG	2.30	0.84
1:C:138:LEU:HD21	1:S:769:GLN:CB	2.05	0.84
1:I:138:LEU:HD23	1:Q:769:GLN:CD	1.98	0.84
2:H:95:LYS:O	2:H:98:THR:HG22	1.78	0.84
2:B:95:LYS:O	2:B:98:THR:HG22	1.78	0.83
2:D:37:ASN:O	5:D:2000:GSP:O2'	2.38	0.83
2:R:95:LYS:O	2:R:98:THR:HG22	1.78	0.83
2:N:95:LYS:O	2:N:98:THR:HG22	1.79	0.83
2:T:95:LYS:O	2:T:98:THR:HG22	1.78	0.83
1:A:138:LEU:HD21	1:O:765:MET:HE2	1.61	0.83
2:P:95:LYS:O	2:P:98:THR:HG22	1.79	0.83
2:B:44:ILE:HB	3:F:737:TYR:CZ	2.14	0.82
2:Z:95:LYS:O	2:Z:98:THR:HG22	1.78	0.82
3:K:738:ILE:HD13	3:L:738:ILE:CG1	2.09	0.82
2:X:95:LYS:O	2:X:98:THR:HG22	1.79	0.82
1:C:138:LEU:HD21	1:W:765:MET:HE3	142.62	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:738:ILE:HG21	3:V:738:ILE:CD1	2.09	0.82
2:J:79:ALA:HB3	3:L:746:MET:CE	2.09	0.82
3:U:731:ASN:HD21	3:V:731:ASN:CG	1.83	0.82
2:D:44:ILE:HD11	3:E:734:LEU:HD22	0.87	0.81
2:J:95:LYS:O	2:J:98:THR:HG22	1.79	0.81
1:M:163:ARG:O	1:M:166:CYS:SG	2.38	0.81
2:D:95:LYS:O	2:D:98:THR:HG22	1.79	0.81
1:A:163:ARG:O	1:A:166:CYS:SG	2.39	0.81
2:D:44:ILE:HD13	3:E:734:LEU:HD22	1.59	0.81
3:F:728:GLU:OE1	3:K:717:ARG:NE	121.26	0.81
1:G:163:ARG:O	1:G:166:CYS:SG	2.39	0.81
1:O:163:ARG:O	1:O:166:CYS:SG	2.39	0.80
1:A:138:LEU:HD11	1:O:765:MET:HE2	1.63	0.80
3:E:724:ILE:CG2	3:V:717:ARG:CZ	2.59	0.80
1:I:138:LEU:HD21	1:Q:765:MET:HG2	1.61	0.80
1:W:163:ARG:O	1:W:166:CYS:SG	2.39	0.80
3:K:738:ILE:HD13	3:L:738:ILE:HG12	1.61	0.80
1:C:163:ARG:O	1:C:166:CYS:SG	2.39	0.80
2:T:44:ILE:CD1	3:V:734:LEU:HD22	2.11	0.80
3:E:717:ARG:NH2	3:V:725:GLN:CB	2.45	0.79
1:G:769:GLN:HB3	1:Y:138:LEU:HD21	181.18	0.79
3:E:717:ARG:HD3	3:V:728:GLU:OE2	1.83	0.79
1:C:138:LEU:CD2	1:S:769:GLN:CD	2.50	0.79
3:E:717:ARG:HG3	3:V:728:GLU:OE1	1.82	0.79
3:F:728:GLU:OE1	3:K:717:ARG:CG	121.02	0.79
1:G:765:MET:HG2	1:Y:138:LEU:CD2	178.73	0.79
1:I:163:ARG:O	1:I:166:CYS:SG	2.39	0.79
1:I:138:LEU:CD2	1:Q:769:GLN:CG	2.60	0.79
3:F:728:GLU:CD	3:K:717:ARG:CG	120.54	0.79
3:E:717:ARG:CG	3:V:728:GLU:CD	2.48	0.79
1:Y:163:ARG:O	1:Y:166:CYS:SG	2.39	0.79
2:D:79:ALA:HB3	3:F:746:MET:CE	2.12	0.79
1:S:163:ARG:O	1:S:166:CYS:SG	2.39	0.79
1:Q:163:ARG:O	1:Q:166:CYS:SG	2.39	0.78
1:I:138:LEU:HD21	1:Q:769:GLN:CB	2.12	0.78
3:E:738:ILE:HG21	3:F:738:ILE:CD1	4.20	0.78
2:D:42:SER:HA	5:D:2000:GSP:S1G	2.78	0.77
3:E:717:ARG:CG	3:V:728:GLU:OE1	2.32	0.77
1:C:331:GLU:CG	1:I:332:GLN:HE22	1.98	0.77
3:K:738:ILE:CD1	3:L:738:ILE:CD1	2.62	0.77
1:M:232:ARG:O	1:M:235:LYS:NZ	2.18	0.77
3:E:717:ARG:CD	3:V:728:GLU:OE2	2.32	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:232:ARG:O	1:O:235:LYS:NZ	2.19	0.76
1:Q:232:ARG:O	1:Q:235:LYS:NZ	2.18	0.76
1:S:232:ARG:O	1:S:235:LYS:NZ	2.18	0.75
3:E:724:ILE:HG23	3:V:717:ARG:CZ	2.16	0.75
1:I:138:LEU:CD2	1:Q:769:GLN:HB3	2.13	0.75
2:T:44:ILE:HD11	3:V:734:LEU:HD21	1.67	0.75
1:C:332:GLN:HE22	1:I:331:GLU:CG	2.00	0.75
1:I:178:GLN:HA	1:I:739:MET:HE1	1.69	0.75
1:Q:178:GLN:HA	1:Q:739:MET:HE1	1.69	0.75
2:B:80:TYR:OH	3:E:746:MET:SD	2.45	0.74
2:B:80:TYR:HH	3:E:746:MET:HG2	1.51	0.74
3:F:734:LEU:HD22	2:R:44:ILE:CD1	120.88	0.74
1:S:178:GLN:HA	1:S:739:MET:HE1	1.70	0.74
2:Z:37:ASN:O	5:Z:2000:GSP:O2'	2.05	0.74
2:D:38:LEU:HA	5:D:2000:GSP:O2'	2.00	0.74
2:B:44:ILE:O	3:F:737:TYR:OH	2.05	0.74
1:I:232:ARG:O	1:I:235:LYS:NZ	2.19	0.74
1:M:178:GLN:HA	1:M:739:MET:HE1	1.70	0.74
3:E:738:ILE:HD13	3:F:738:ILE:CG1	2.18	0.74
1:C:178:GLN:HA	1:C:739:MET:HE1	1.70	0.73
1:C:232:ARG:O	1:C:235:LYS:NZ	2.19	0.73
2:D:44:ILE:CD1	3:E:734:LEU:CD2	2.27	0.73
2:J:79:ALA:CB	3:L:746:MET:HE3	2.17	0.73
1:O:178:GLN:HA	1:O:739:MET:HE1	1.70	0.73
1:S:393:ASN:O	1:S:397:THR:OG1	2.07	0.73
1:W:232:ARG:O	1:W:235:LYS:NZ	2.19	0.73
3:E:735:GLN:NE2	3:F:734:LEU:CD1	3.83	0.73
1:G:178:GLN:HA	1:G:739:MET:HE1	1.70	0.73
3:E:735:GLN:NE2	3:F:734:LEU:HD12	4.28	0.73
3:F:728:GLU:CD	3:K:717:ARG:HG3	119.60	0.73
1:Q:393:ASN:O	1:Q:397:THR:OG1	2.07	0.73
3:E:717:ARG:HD2	3:V:724:ILE:HG22	1.71	0.73
1:Y:232:ARG:O	1:Y:235:LYS:NZ	2.19	0.73
1:Y:178:GLN:HA	1:Y:739:MET:HE1	1.69	0.73
1:C:332:GLN:HE21	1:I:332:GLN:HG3	1.53	0.73
1:G:769:GLN:HB3	1:Y:138:LEU:CD2	180.40	0.73
1:I:138:LEU:CD2	1:Q:769:GLN:CD	2.57	0.72
1:G:232:ARG:O	1:G:235:LYS:NZ	2.19	0.72
1:C:393:ASN:O	1:C:397:THR:OG1	2.07	0.72
2:B:44:ILE:HD12	3:F:737:TYR:CD2	2.24	0.72
1:O:393:ASN:O	1:O:397:THR:OG1	2.07	0.72
1:W:393:ASN:O	1:W:397:THR:OG1	2.08	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:393:ASN:O	1:A:397:THR:OG1	2.07	0.72
1:G:393:ASN:O	1:G:397:THR:OG1	2.07	0.72
1:W:178:GLN:HA	1:W:739:MET:HE1	1.72	0.72
1:M:393:ASN:O	1:M:397:THR:OG1	2.07	0.72
3:E:717:ARG:HD2	3:V:724:ILE:CG2	2.20	0.72
1:I:393:ASN:O	1:I:397:THR:OG1	2.07	0.72
2:D:40:SER:HB3	5:D:2000:GSP:H3'	1.99	0.71
1:A:178:GLN:HA	1:A:739:MET:HE1	1.71	0.71
1:Y:393:ASN:O	1:Y:397:THR:OG1	2.07	0.71
3:F:728:GLU:OE1	3:K:717:ARG:HG3	120.08	0.71
2:T:44:ILE:CD1	3:V:734:LEU:CD2	2.69	0.71
1:A:232:ARG:O	1:A:235:LYS:NZ	2.19	0.71
1:C:138:LEU:HD21	1:W:765:MET:HE2	142.50	0.71
2:J:44:ILE:HD11	3:K:734:LEU:HD22	0.73	0.71
3:E:724:ILE:O	3:V:717:ARG:NH1	2.24	0.70
2:T:44:ILE:HD13	3:V:734:LEU:HD22	1.73	0.70
2:H:44:ILE:HB	3:L:737:TYR:CZ	2.26	0.70
1:C:138:LEU:CD2	1:S:769:GLN:CB	2.68	0.70
3:F:728:GLU:OE2	3:K:717:ARG:HG3	118.56	0.70
3:U:731:ASN:ND2	3:V:731:ASN:CG	2.45	0.70
2:P:38:LEU:O	5:P:2000:GSP:O3'	2.10	0.70
3:E:738:ILE:HD13	3:F:738:ILE:CD1	2.21	0.70
3:K:738:ILE:CD1	3:L:738:ILE:HD13	2.22	0.69
2:D:79:ALA:CB	3:F:746:MET:HE1	2.20	0.69
2:B:80:TYR:OH	3:E:746:MET:CB	2.41	0.69
3:E:717:ARG:NH2	3:L:731:ASN:HD22	123.12	0.69
1:C:139:PHE:HA	1:C:143:MET:HE2	1.76	0.69
2:J:44:ILE:CD1	3:K:734:LEU:CD2	2.17	0.69
3:F:734:LEU:CD2	2:R:44:ILE:CD1	120.43	0.68
1:Q:139:PHE:HA	1:Q:143:MET:HE2	1.75	0.68
2:B:38:LEU:HA	5:B:2000:GSP:O2'	1.94	0.68
1:C:332:GLN:HG3	1:I:332:GLN:CG	2.24	0.68
1:S:139:PHE:HA	1:S:143:MET:HE2	1.76	0.68
1:A:139:PHE:HA	1:A:143:MET:HE2	1.75	0.67
1:C:221:SER:C	2:Z:71:GLU:OE2	125.72	0.67
2:J:79:ALA:HB1	3:L:746:MET:HE3	1.76	0.67
1:O:139:PHE:HA	1:O:143:MET:HE2	1.74	0.67
1:G:139:PHE:HA	1:G:143:MET:HE2	1.75	0.67
1:Y:139:PHE:HA	1:Y:143:MET:HE2	1.75	0.67
2:J:38:LEU:HA	5:J:2000:GSP:O2'	1.94	0.67
3:E:717:ARG:HH21	3:V:725:GLN:CB	2.04	0.67
3:F:717:ARG:NH1	3:K:724:ILE:O	120.35	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:717:ARG:NH1	3:K:728:GLU:HB2	123.05	0.67
1:I:139:PHE:HA	1:I:143:MET:HE2	1.76	0.67
1:M:139:PHE:HA	1:M:143:MET:HE2	1.76	0.67
1:W:139:PHE:HA	1:W:143:MET:HE2	1.76	0.67
2:D:79:ALA:HB1	3:F:746:MET:HE3	1.77	0.66
2:N:38:LEU:O	5:N:2000:GSP:O3'	2.13	0.66
1:C:138:LEU:CG	1:S:769:GLN:CB	2.73	0.66
3:U:738:ILE:HD13	3:V:738:ILE:CD1	2.22	0.66
1:C:138:LEU:HD23	1:S:769:GLN:OE1	1.95	0.66
2:D:79:ALA:HB3	3:F:746:MET:HE3	1.72	0.66
3:E:752:ILE:HG21	3:F:745:ILE:HD11	3.84	0.65
3:E:742:ILE:HD11	3:F:741:ILE:HG21	1.79	0.65
3:K:738:ILE:HD13	3:L:738:ILE:HD11	1.73	0.65
1:C:138:LEU:HD11	1:W:765:MET:HE2	144.78	0.65
2:H:44:ILE:O	3:L:737:TYR:OH	2.15	0.65
2:N:38:LEU:HA	5:N:2000:GSP:O2'	1.96	0.65
2:T:26:ASN:ND2	5:T:2000:GSP:O1A	2.29	0.65
1:G:769:GLN:CB	1:Y:138:LEU:HG	181.93	0.64
3:E:738:ILE:CD1	3:F:738:ILE:HD13	2.56	0.64
3:F:725:GLN:CB	3:K:717:ARG:NH2	122.43	0.64
2:Z:45:GLY:O	2:Z:67:THR:O	2.16	0.64
2:H:45:GLY:O	2:H:67:THR:O	2.16	0.64
2:N:45:GLY:O	2:N:67:THR:O	2.16	0.64
2:P:40:SER:HB3	5:P:2000:GSP:H3'	1.79	0.64
2:P:45:GLY:O	2:P:67:THR:O	2.16	0.64
2:T:80:TYR:OH	3:U:746:MET:HB3	1.98	0.64
2:X:45:GLY:O	2:X:67:THR:O	2.16	0.64
2:R:45:GLY:O	2:R:67:THR:O	2.16	0.63
2:D:79:ALA:HB3	3:F:746:MET:HE1	1.78	0.63
2:B:80:TYR:CE1	3:E:746:MET:HE1	2.33	0.63
2:T:45:GLY:O	2:T:67:THR:O	2.16	0.63
2:D:45:GLY:O	2:D:67:THR:O	2.16	0.63
1:Y:618:TYR:CZ	1:Y:622:GLU:HG3	2.33	0.63
2:J:45:GLY:O	2:J:67:THR:O	2.16	0.63
2:B:45:GLY:O	2:B:67:THR:O	2.16	0.63
3:F:724:ILE:HG22	3:K:717:ARG:CD	118.88	0.63
1:C:221:SER:HA	2:P:71:GLU:OE2	1.99	0.62
2:B:81:TYR:HB3	2:B:113:ALA:HB2	1.82	0.62
2:H:67:THR:O	2:H:68:ALA:HB3	2.00	0.62
1:Q:618:TYR:CZ	1:Q:622:GLU:HG3	2.35	0.62
1:S:618:TYR:CZ	1:S:622:GLU:HG3	2.35	0.62
1:G:765:MET:HA	1:G:769:GLN:OE1	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:138:LEU:CD2	1:Q:769:GLN:CB	2.75	0.62
1:A:138:LEU:CD1	1:O:765:MET:HE2	2.30	0.62
2:Z:67:THR:O	2:Z:68:ALA:HB3	2.00	0.62
1:C:221:SER:C	2:P:71:GLU:OE2	2.37	0.62
2:D:81:TYR:HB3	2:D:113:ALA:HB2	1.82	0.62
1:I:221:SER:HA	2:N:71:GLU:OE2	1.99	0.62
2:B:67:THR:O	2:B:68:ALA:HB3	2.00	0.62
2:D:26:ASN:ND2	5:D:2000:GSP:O1A	2.36	0.62
1:Q:765:MET:HA	1:Q:769:GLN:OE1	1.99	0.62
3:F:731:ASN:HD22	3:U:717:ARG:NH2	1.98	0.62
2:H:44:ILE:HD12	3:L:737:TYR:CD2	2.35	0.61
2:P:67:THR:O	2:P:68:ALA:HB3	2.00	0.61
1:O:765:MET:HA	1:O:769:GLN:OE1	1.99	0.61
2:X:81:TYR:HB3	2:X:113:ALA:HB2	1.82	0.61
1:Y:626:TYR:HA	1:Y:631:PHE:CD1	2.35	0.61
2:R:67:THR:O	2:R:68:ALA:HB3	2.00	0.61
2:D:67:THR:O	2:D:68:ALA:HB3	2.01	0.61
3:E:731:ASN:ND2	3:F:731:ASN:ND2	5.29	0.61
2:J:67:THR:O	2:J:68:ALA:HB3	2.01	0.61
1:C:765:MET:HE2	1:W:138:LEU:HD11	141.92	0.61
2:N:67:THR:O	2:N:68:ALA:HB3	2.00	0.61
1:M:765:MET:HA	1:M:769:GLN:OE1	2.00	0.61
2:T:67:THR:O	2:T:68:ALA:HB3	2.00	0.61
2:H:71:GLU:OE2	1:W:221:SER:C	118.62	0.61
1:W:765:MET:HA	1:W:769:GLN:OE1	2.00	0.61
1:Y:765:MET:HA	1:Y:769:GLN:OE1	2.01	0.61
2:Z:38:LEU:O	5:Z:2000:GSP:O3'	2.16	0.61
3:F:734:LEU:HD22	2:R:44:ILE:HD13	120.79	0.61
2:H:81:TYR:HB3	2:H:113:ALA:HB2	1.83	0.61
1:A:626:TYR:HA	1:A:631:PHE:CD1	2.35	0.61
1:G:618:TYR:CZ	1:G:622:GLU:HG3	2.36	0.61
2:J:81:TYR:HB3	2:J:113:ALA:HB2	1.82	0.61
2:P:38:LEU:HA	5:P:2000:GSP:O2'	2.01	0.61
2:R:81:TYR:HB3	2:R:113:ALA:HB2	1.82	0.61
2:B:80:TYR:CE1	3:E:746:MET:SD	2.94	0.61
1:G:626:TYR:HA	1:G:631:PHE:CD2	2.35	0.61
1:I:134:PHE:O	1:I:163:ARG:NH1	2.34	0.61
1:W:618:TYR:CZ	1:W:622:GLU:HG3	2.35	0.61
1:Y:134:PHE:O	1:Y:163:ARG:NH1	2.34	0.61
1:S:765:MET:HA	1:S:769:GLN:OE1	2.00	0.61
2:T:81:TYR:HB3	2:T:113:ALA:HB2	1.82	0.61
1:C:134:PHE:O	1:C:163:ARG:NH1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:637:ASN:HB3	1:C:669:HIS:CD2	2.37	0.60
2:X:67:THR:O	2:X:68:ALA:HB3	2.01	0.60
1:A:765:MET:HA	1:A:769:GLN:OE1	2.01	0.60
2:D:80:TYR:CE1	3:F:746:MET:HG2	2.36	0.60
1:M:637:ASN:HB3	1:M:669:HIS:CD2	2.37	0.60
1:A:618:TYR:CZ	1:A:622:GLU:HG3	2.36	0.60
1:C:759:GLU:OE2	1:S:147:TYR:OH	2.19	0.60
1:I:637:ASN:HB3	1:I:669:HIS:CD2	2.37	0.60
1:W:637:ASN:HB3	1:W:669:HIS:CD2	2.36	0.60
1:Y:637:ASN:HB3	1:Y:669:HIS:CD2	2.37	0.60
1:C:765:MET:HA	1:C:769:GLN:OE1	2.01	0.60
2:N:81:TYR:HB3	2:N:113:ALA:HB2	1.82	0.60
3:E:717:ARG:NE	3:V:728:GLU:OE1	2.35	0.60
1:A:134:PHE:O	1:A:163:ARG:NH1	2.35	0.60
1:A:765:MET:CE	1:O:138:LEU:HD21	2.32	0.60
1:I:765:MET:HA	1:I:769:GLN:OE1	2.01	0.60
1:C:618:TYR:CZ	1:C:622:GLU:HG3	2.39	0.60
3:K:742:ILE:HD11	3:L:741:ILE:HG21	1.82	0.60
2:Z:81:TYR:HB3	2:Z:113:ALA:HB2	1.82	0.60
2:Z:25:SER:HG	6:Z:2001:MG:MG	1.10	0.60
3:E:724:ILE:HG22	3:V:717:ARG:CZ	2.31	0.60
2:H:38:LEU:HA	5:H:2000:GSP:O2'	2.01	0.60
1:G:765:MET:CE	1:M:138:LEU:HD21	2.32	0.60
1:Q:637:ASN:HB3	1:Q:669:HIS:CD2	2.37	0.60
1:G:637:ASN:HB3	1:G:669:HIS:CD2	2.37	0.60
1:M:134:PHE:O	1:M:163:ARG:NH1	2.35	0.60
1:G:134:PHE:O	1:G:163:ARG:NH1	2.35	0.59
1:A:637:ASN:HB3	1:A:669:HIS:CD2	2.36	0.59
2:P:42:SER:HA	5:P:2000:GSP:S1G	2.43	0.59
2:X:40:SER:HB3	5:X:2000:GSP:H3'	1.83	0.59
1:G:765:MET:CG	1:Y:138:LEU:HD21	179.02	0.59
1:O:637:ASN:HB3	1:O:669:HIS:CD2	2.38	0.59
2:P:81:TYR:HB3	2:P:113:ALA:HB2	1.83	0.59
1:C:138:LEU:CD2	1:S:765:MET:HG2	2.27	0.59
1:C:332:GLN:NE2	1:I:331:GLU:HG3	2.15	0.59
1:I:618:TYR:CZ	1:I:622:GLU:HG3	2.38	0.59
2:X:38:LEU:O	5:X:2000:GSP:O3'	2.18	0.59
2:B:80:TYR:OH	3:E:746:MET:HB3	2.04	0.58
1:G:138:LEU:HD11	1:M:765:MET:HE2	1.83	0.58
1:Q:134:PHE:O	1:Q:163:ARG:NH1	2.36	0.58
1:S:637:ASN:HB3	1:S:669:HIS:CD2	2.38	0.58
1:C:332:GLN:CG	1:I:332:GLN:HG2	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:134:PHE:O	1:O:163:ARG:NH1	2.36	0.58
1:Q:626:TYR:HA	1:Q:631:PHE:CD2	2.38	0.58
2:T:38:LEU:HA	5:T:2000:GSP:O2'	2.03	0.58
2:B:42:SER:HA	5:B:2000:GSP:S1G	2.43	0.58
2:N:40:SER:HB3	5:N:2000:GSP:H3'	1.85	0.58
1:C:332:GLN:CG	1:I:332:GLN:CG	2.82	0.58
1:C:765:MET:CE	1:W:138:LEU:HD11	142.46	0.58
1:C:332:GLN:HG3	1:I:332:GLN:HG3	1.85	0.58
1:S:626:TYR:HA	1:S:631:PHE:CD1	2.38	0.58
1:A:625:SER:O	1:A:628:THR:HG22	2.04	0.58
1:C:625:SER:O	1:C:628:THR:HG22	2.05	0.58
1:G:769:GLN:HB3	1:Y:138:LEU:CG	180.73	0.58
1:S:134:PHE:O	1:S:163:ARG:NH1	2.37	0.58
1:Y:625:SER:O	1:Y:628:THR:HG22	2.03	0.58
1:M:618:TYR:CZ	1:M:622:GLU:HG3	2.40	0.57
1:S:625:SER:O	1:S:628:THR:HG22	2.04	0.57
1:W:134:PHE:O	1:W:163:ARG:NH1	2.37	0.57
1:G:625:SER:O	1:G:628:THR:HG22	2.04	0.57
1:O:618:TYR:CZ	1:O:622:GLU:HG3	2.40	0.57
1:G:138:LEU:CD2	1:M:765:MET:HE3	2.26	0.57
2:J:26:ASN:ND2	5:J:2000:GSP:O1A	2.37	0.57
1:Q:625:SER:O	1:Q:628:THR:HG22	2.04	0.57
1:C:138:LEU:HG	1:S:769:GLN:CB	2.28	0.57
1:G:626:TYR:HA	1:G:631:PHE:CD1	3.46	0.57
2:H:40:SER:HB3	5:H:2000:GSP:H3'	2.03	0.57
1:M:626:TYR:HA	1:M:631:PHE:CD1	2.40	0.57
2:N:42:SER:HA	5:N:2000:GSP:S1G	2.45	0.57
1:G:611:SER:HB2	1:G:613:LEU:HD22	1.87	0.57
1:M:625:SER:O	1:M:628:THR:HG22	2.04	0.57
1:C:765:MET:CE	1:W:138:LEU:HD21	140.02	0.57
1:W:626:TYR:HA	1:W:631:PHE:CD1	2.40	0.57
2:H:42:SER:HA	5:H:2000:GSP:S1G	2.56	0.57
1:W:625:SER:O	1:W:628:THR:HG22	2.04	0.57
1:C:329:THR:HG21	1:I:329:THR:HG21	1.86	0.56
1:C:221:SER:CA	2:P:71:GLU:OE2	2.53	0.56
3:E:735:GLN:NE2	3:F:734:LEU:HD13	2.86	0.56
1:O:625:SER:O	1:O:628:THR:HG22	2.04	0.56
1:C:332:GLN:HG2	1:I:332:GLN:HG2	1.87	0.56
1:I:625:SER:O	1:I:628:THR:HG22	2.05	0.56
1:I:138:LEU:CG	1:Q:769:GLN:CB	2.84	0.56
1:I:611:SER:HB2	1:I:613:LEU:HD22	1.88	0.56
1:C:611:SER:HB2	1:C:613:LEU:HD22	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:626:TYR:HA	1:O:631:PHE:CD1	2.41	0.56
1:A:611:SER:HB2	1:A:613:LEU:HD22	1.88	0.56
1:M:611:SER:HB2	1:M:613:LEU:HD22	1.88	0.56
2:X:38:LEU:HA	5:X:2000:GSP:O2'	2.05	0.56
2:H:38:LEU:O	5:H:2000:GSP:O3'	2.20	0.56
2:J:80:TYR:CE1	3:L:746:MET:HG2	2.40	0.56
2:P:144:GLU:OE1	2:P:144:GLU:HA	2.06	0.56
2:D:144:GLU:OE1	2:D:144:GLU:HA	2.07	0.56
2:N:144:GLU:OE1	2:N:144:GLU:HA	2.06	0.56
2:D:25:SER:OG	5:D:2000:GSP:O2B	2.74	0.55
3:E:731:ASN:ND2	3:F:731:ASN:OD1	3.21	0.55
1:Y:611:SER:HB2	1:Y:613:LEU:HD22	1.88	0.55
1:I:626:TYR:HA	1:I:631:PHE:CD1	2.40	0.55
3:E:725:GLN:HA	3:L:717:ARG:NH2	119.09	0.55
2:J:144:GLU:HA	2:J:144:GLU:OE1	2.06	0.55
2:X:144:GLU:OE1	2:X:144:GLU:HA	2.07	0.55
2:Z:40:SER:HB3	5:Z:2000:GSP:H3'	1.87	0.55
2:B:144:GLU:HA	2:B:144:GLU:OE1	2.07	0.55
1:W:611:SER:HB2	1:W:613:LEU:HD22	1.87	0.55
1:G:138:LEU:CD1	1:M:765:MET:HE2	2.37	0.55
1:O:611:SER:HB2	1:O:613:LEU:HD22	1.89	0.55
2:B:80:TYR:HE1	3:E:746:MET:SD	2.30	0.55
2:H:144:GLU:HA	2:H:144:GLU:OE1	2.07	0.55
3:E:717:ARG:HD3	3:V:724:ILE:HG22	1.85	0.55
1:S:611:SER:HB2	1:S:613:LEU:HD22	1.88	0.55
1:I:138:LEU:HD23	1:Q:769:GLN:OE1	2.06	0.55
1:C:607:VAL:O	1:C:611:SER:OG	2.20	0.55
1:Q:611:SER:HB2	1:Q:613:LEU:HD22	1.88	0.55
3:E:717:ARG:CD	3:V:724:ILE:CG2	2.77	0.54
1:O:196:PRO:HG2	2:P:131:LEU:HD22	1.89	0.54
2:T:144:GLU:HA	2:T:144:GLU:OE1	2.07	0.54
2:Z:144:GLU:HA	2:Z:144:GLU:OE1	2.07	0.54
3:E:717:ARG:NH2	3:V:725:GLN:CA	2.71	0.54
3:E:717:ARG:NH2	3:L:728:GLU:CG	122.08	0.54
1:O:133:LEU:O	1:O:136:SER:OG	2.21	0.54
2:B:38:LEU:O	5:B:2000:GSP:O3'	2.14	0.54
2:R:125:LYS:HG2	5:R:2000:GSP:C6	2.42	0.54
2:B:40:SER:HB3	5:B:2000:GSP:H3'	1.89	0.54
2:H:125:LYS:HG2	5:H:2000:GSP:C6	2.58	0.54
1:M:133:LEU:O	1:M:136:SER:OG	2.21	0.54
2:R:144:GLU:OE1	2:R:144:GLU:HA	2.07	0.54
1:C:626:TYR:HA	1:C:631:PHE:CD1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:717:ARG:CZ	3:K:724:ILE:CG2	119.60	0.53
3:E:717:ARG:NH2	3:L:728:GLU:HG2	122.21	0.53
1:M:196:PRO:HG2	2:N:131:LEU:HD22	1.89	0.53
2:H:80:TYR:OH	3:K:746:MET:CB	2.56	0.53
1:M:306:ARG:O	1:M:351:ARG:NH1	2.41	0.53
1:O:306:ARG:O	1:O:351:ARG:NH1	2.41	0.53
2:H:8:TYR:HA	2:H:59:THR:OG1	2.10	0.53
1:Q:602:VAL:HG23	1:Q:607:VAL:HG23	1.90	0.53
2:X:8:TYR:HA	2:X:59:THR:OG1	2.08	0.53
1:C:602:VAL:HG23	1:C:607:VAL:HG23	1.92	0.53
3:E:724:ILE:HG23	3:V:717:ARG:NH2	2.23	0.53
2:D:8:TYR:CE2	2:D:11:LEU:HB2	2.47	0.53
1:C:331:GLU:HG3	1:I:332:GLN:HE22	1.73	0.53
1:I:602:VAL:HG23	1:I:607:VAL:HG23	1.91	0.53
2:Z:67:THR:O	2:Z:68:ALA:CB	2.57	0.53
1:M:602:VAL:HG23	1:M:607:VAL:HG23	1.91	0.53
2:R:8:TYR:HA	2:R:59:THR:OG1	2.09	0.53
2:H:67:THR:O	2:H:68:ALA:CB	2.57	0.53
1:S:306:ARG:O	1:S:351:ARG:NH1	2.42	0.53
2:R:40:SER:HB3	5:R:2000:GSP:H3'	1.91	0.52
1:S:602:VAL:HG23	1:S:607:VAL:HG23	1.90	0.52
5:X:2000:GSP:O2B	5:X:2000:GSP:O3G	2.27	0.52
5:D:2000:GSP:O2B	5:D:2000:GSP:O3G	2.29	0.52
1:A:306:ARG:O	1:A:351:ARG:NH1	2.42	0.52
2:N:8:TYR:CE2	2:N:11:LEU:HB2	2.44	0.52
2:P:8:TYR:CE2	2:P:11:LEU:HB2	2.44	0.52
2:R:92:ASP:H	2:R:98:THR:HG21	1.74	0.52
5:T:2000:GSP:O2B	5:T:2000:GSP:O3G	2.27	0.52
2:D:92:ASP:H	2:D:98:THR:HG21	1.74	0.52
1:G:306:ARG:O	1:G:351:ARG:NH1	2.42	0.52
2:H:26:ASN:ND2	5:H:2000:GSP:O1A	2.40	0.52
1:O:602:VAL:HG23	1:O:607:VAL:HG23	1.92	0.52
2:T:8:TYR:HA	2:T:59:THR:OG1	2.10	0.52
2:X:67:THR:O	2:X:68:ALA:CB	2.58	0.52
1:A:765:MET:HE3	1:O:138:LEU:HD21	1.91	0.52
1:G:133:LEU:O	1:G:136:SER:OG	2.21	0.52
3:U:735:GLN:NE2	3:V:734:LEU:CD1	2.72	0.52
1:W:306:ARG:O	1:W:351:ARG:NH1	2.43	0.52
2:Z:8:TYR:CE2	2:Z:11:LEU:HB2	2.45	0.52
1:A:138:LEU:CD2	1:O:765:MET:HE2	2.31	0.52
1:A:602:VAL:HG23	1:A:607:VAL:HG23	1.92	0.52
2:D:67:THR:O	2:D:68:ALA:CB	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:138:LEU:CD2	1:W:765:MET:CE	143.28	0.52
2:P:26:ASN:ND2	5:P:2000:GSP:O1A	2.39	0.52
1:Q:306:ARG:O	1:Q:351:ARG:NH1	2.42	0.52
1:Q:628:THR:HG23	1:Q:631:PHE:H	1.75	0.52
1:A:133:LEU:O	1:A:136:SER:OG	2.21	0.52
1:C:138:LEU:CG	1:S:769:GLN:CD	2.79	0.52
2:R:67:THR:O	2:R:68:ALA:CB	2.57	0.52
5:Z:2000:GSP:O2B	5:Z:2000:GSP:O3G	2.27	0.52
2:H:92:ASP:H	2:H:98:THR:HG21	1.75	0.52
2:N:8:TYR:HA	2:N:59:THR:OG1	2.09	0.52
1:I:138:LEU:CD2	1:Q:765:MET:HG2	2.35	0.52
1:C:138:LEU:CD2	1:W:765:MET:HE3	142.95	0.52
1:Y:306:ARG:O	1:Y:351:ARG:NH1	2.43	0.52
1:C:306:ARG:O	1:C:351:ARG:NH1	2.43	0.52
2:D:8:TYR:HA	2:D:59:THR:OG1	2.11	0.52
5:H:2000:GSP:O3G	5:H:2000:GSP:O2B	2.27	0.52
1:I:306:ARG:O	1:I:351:ARG:NH1	2.43	0.52
1:G:765:MET:HE3	1:M:138:LEU:HD21	1.91	0.52
2:T:67:THR:O	2:T:68:ALA:CB	2.57	0.52
3:U:738:ILE:CD1	3:V:738:ILE:HD13	2.26	0.52
1:Y:602:VAL:HG23	1:Y:607:VAL:HG23	1.92	0.52
2:B:67:THR:O	2:B:68:ALA:CB	2.57	0.51
3:E:738:ILE:CD1	3:F:738:ILE:CD1	2.88	0.51
2:J:8:TYR:HA	2:J:59:THR:OG1	2.09	0.51
2:N:26:ASN:ND2	5:N:2000:GSP:O1A	2.41	0.51
2:P:8:TYR:HA	2:P:59:THR:OG1	2.09	0.51
1:S:196:PRO:HG2	2:T:131:LEU:HD22	1.92	0.51
1:G:602:VAL:HG23	1:G:607:VAL:HG23	1.93	0.51
2:H:8:TYR:CE2	2:H:11:LEU:HB2	2.47	0.51
1:S:628:THR:HG23	1:S:631:PHE:H	1.75	0.51
1:W:602:VAL:HG23	1:W:607:VAL:HG23	1.91	0.51
2:Z:92:ASP:H	2:Z:98:THR:HG21	1.75	0.51
2:J:67:THR:O	2:J:68:ALA:CB	2.58	0.51
1:A:765:MET:HE2	1:O:138:LEU:HD11	1.92	0.51
1:I:206:ILE:HD11	1:I:394:PHE:HE2	1.75	0.51
2:P:67:THR:O	2:P:68:ALA:CB	2.57	0.51
1:W:628:THR:HG23	1:W:631:PHE:H	1.75	0.51
1:Q:133:LEU:O	1:Q:136:SER:OG	2.21	0.51
1:C:138:LEU:CG	1:S:769:GLN:HB3	2.40	0.51
2:Z:26:ASN:ND2	5:Z:2000:GSP:O1A	2.43	0.51
2:Z:8:TYR:HA	2:Z:59:THR:OG1	2.10	0.51
3:E:738:ILE:CD1	3:F:738:ILE:HG12	2.33	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:92:ASP:H	2:P:98:THR:HG21	1.76	0.51
1:S:133:LEU:O	1:S:136:SER:OG	2.21	0.51
2:X:8:TYR:CE2	2:X:11:LEU:HB2	2.46	0.51
2:X:92:ASP:H	2:X:98:THR:HG21	1.74	0.51
2:B:8:TYR:HA	2:B:59:THR:OG1	2.10	0.51
1:G:628:THR:HG23	1:G:631:PHE:H	1.75	0.51
2:B:92:ASP:H	2:B:98:THR:HG21	1.76	0.51
1:C:331:GLU:CB	1:I:332:GLN:HE22	2.23	0.51
3:K:738:ILE:CD1	3:L:738:ILE:HG12	2.35	0.51
3:E:717:ARG:HH21	3:L:728:GLU:HG2	121.37	0.51
2:N:67:THR:O	2:N:68:ALA:CB	2.57	0.51
2:N:92:ASP:H	2:N:98:THR:HG21	1.76	0.51
2:X:125:LYS:HG2	5:X:2000:GSP:C6	2.46	0.51
1:A:178:GLN:CD	1:A:739:MET:CE	2.79	0.51
1:M:607:VAL:O	1:M:611:SER:OG	2.20	0.51
2:X:42:SER:HA	5:X:2000:GSP:S1G	2.51	0.51
1:Y:628:THR:HG23	1:Y:631:PHE:H	1.77	0.51
2:T:8:TYR:CE2	2:T:11:LEU:HB2	2.45	0.50
1:W:133:LEU:O	1:W:136:SER:OG	2.21	0.50
1:A:628:THR:HG23	1:A:631:PHE:H	1.76	0.50
3:F:717:ARG:CZ	3:K:724:ILE:HG22	119.79	0.50
5:N:2000:GSP:O2B	5:N:2000:GSP:O3G	2.28	0.50
1:O:607:VAL:O	1:O:611:SER:OG	2.20	0.50
1:W:356:THR:HG21	1:W:546:VAL:HG12	1.93	0.50
1:C:206:ILE:HD11	1:C:394:PHE:HE2	1.75	0.50
2:D:91:TYR:HB2	2:D:98:THR:HG23	1.94	0.50
3:E:717:ARG:NH2	3:L:728:GLU:HA	123.77	0.50
2:R:8:TYR:CE2	2:R:11:LEU:HB2	2.46	0.50
2:T:92:ASP:H	2:T:98:THR:HG21	1.76	0.50
1:G:196:PRO:HG2	2:H:131:LEU:HD22	1.98	0.50
1:Q:356:THR:HG21	1:Q:546:VAL:HG12	1.93	0.50
5:B:2000:GSP:O2B	5:B:2000:GSP:O3G	2.29	0.49
3:K:720:LEU:O	3:K:724:ILE:HG12	2.11	0.49
1:O:628:THR:HG23	1:O:631:PHE:H	1.77	0.49
5:P:2000:GSP:O3G	5:P:2000:GSP:O2B	2.29	0.49
5:R:2000:GSP:O2B	5:R:2000:GSP:O3G	2.30	0.49
1:I:628:THR:HG23	1:I:631:PHE:H	1.76	0.49
3:E:728:GLU:CB	3:L:717:ARG:NH2	123.87	0.49
1:S:356:THR:HG21	1:S:546:VAL:HG12	1.94	0.49
1:M:518:LEU:HG	1:M:519:LYS:H	1.77	0.49
1:M:628:THR:HG23	1:M:631:PHE:H	1.78	0.49
3:E:717:ARG:HH21	3:L:728:GLU:HA	122.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:724:ILE:HG22	3:K:717:ARG:HD2	119.85	0.49
2:N:120:MET:HE3	2:N:164:ALA:HB1	1.95	0.49
1:O:356:THR:HG21	1:O:546:VAL:HG12	1.95	0.49
2:B:91:TYR:HB2	2:B:98:THR:HG23	1.95	0.49
1:C:628:THR:HG23	1:C:631:PHE:H	1.76	0.49
2:J:91:TYR:HB2	2:J:98:THR:HG23	1.95	0.49
1:G:356:THR:HG21	1:G:546:VAL:HG12	1.95	0.49
1:G:518:LEU:HG	1:G:519:LYS:H	1.80	0.49
1:W:611:SER:HB2	1:W:613:LEU:CD2	2.43	0.49
1:A:138:LEU:HD21	1:O:765:MET:SD	2.50	0.49
1:I:356:THR:HG21	1:I:546:VAL:HG12	1.95	0.49
2:H:91:TYR:HB2	2:H:98:THR:HG23	1.95	0.49
1:G:769:GLN:HB3	1:Y:138:LEU:HG	181.02	0.49
2:D:120:MET:HB2	2:D:168:ILE:HD12	1.95	0.48
3:F:725:GLN:CB	3:K:717:ARG:HH21	121.58	0.48
1:Q:607:VAL:O	1:Q:611:SER:OG	2.20	0.48
3:E:717:ARG:HD2	3:V:724:ILE:HG21	1.94	0.48
1:I:611:SER:HB2	1:I:613:LEU:CD2	2.43	0.48
2:J:92:ASP:H	2:J:98:THR:HG21	1.78	0.48
1:M:178:GLN:CD	1:M:739:MET:CE	2.81	0.48
1:M:768:GLU:CD	1:M:768:GLU:H	2.17	0.48
1:S:766:THR:HG22	1:S:769:GLN:HG3	1.95	0.48
3:U:735:GLN:NE2	3:V:734:LEU:HD12	2.27	0.48
1:G:611:SER:HB2	1:G:613:LEU:CD2	2.43	0.48
1:M:206:ILE:HD11	1:M:394:PHE:HE2	1.77	0.48
2:P:120:MET:HE3	2:P:164:ALA:HB1	1.95	0.48
1:A:356:THR:HG21	1:A:546:VAL:HG12	1.95	0.48
2:B:8:TYR:CE2	2:B:11:LEU:HB2	2.48	0.48
1:C:611:SER:HB2	1:C:613:LEU:CD2	2.44	0.48
3:E:752:ILE:HG21	3:F:745:ILE:CD1	3.88	0.48
1:I:518:LEU:HG	1:I:519:LYS:H	1.79	0.48
1:M:518:LEU:HG	1:M:519:LYS:N	2.29	0.48
1:I:221:SER:CA	2:N:71:GLU:OE2	2.61	0.48
1:Q:766:THR:HG22	1:Q:769:GLN:HG3	1.95	0.48
3:E:729:GLU:HG3	1:S:751:SER:OG	2.13	0.48
2:T:42:SER:HA	5:T:2000:GSP:S1G	2.53	0.48
3:E:720:LEU:O	3:E:724:ILE:HG12	2.12	0.48
2:J:38:LEU:O	5:J:2000:GSP:O3'	2.22	0.48
2:P:91:TYR:HB2	2:P:98:THR:HG23	1.95	0.48
2:R:91:TYR:HB2	2:R:98:THR:HG23	1.94	0.48
1:C:206:ILE:HD11	1:C:394:PHE:HE1	5.52	0.48
2:N:91:TYR:HB2	2:N:98:THR:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:206:ILE:HD11	1:W:394:PHE:HE2	1.79	0.48
3:E:717:ARG:NH2	3:L:731:ASN:ND2	123.23	0.48
1:O:768:GLU:H	1:O:768:GLU:CD	2.17	0.48
1:S:607:VAL:O	1:S:611:SER:OG	2.20	0.48
1:S:611:SER:HB2	1:S:613:LEU:CD2	2.43	0.48
2:X:91:TYR:HB2	2:X:98:THR:HG23	1.95	0.48
1:Y:206:ILE:HD11	1:Y:394:PHE:HE1	1.79	0.48
2:B:120:MET:HB2	2:B:168:ILE:HD12	1.96	0.48
3:L:720:LEU:O	3:L:724:ILE:HG13	2.14	0.48
1:M:356:THR:HG21	1:M:546:VAL:HG12	1.96	0.48
1:S:588:ILE:HD12	1:S:593:GLY:HA2	1.95	0.48
1:Y:356:THR:HG21	1:Y:546:VAL:HG12	1.96	0.48
2:B:120:MET:HE1	2:B:164:ALA:HB1	1.95	0.48
1:C:518:LEU:HG	1:C:519:LYS:H	1.79	0.48
1:G:182:MET:HA	1:G:186:MET:HG3	1.97	0.48
1:I:178:GLN:CA	1:I:739:MET:HE1	2.42	0.48
2:J:8:TYR:CE2	2:J:11:LEU:HB2	2.48	0.48
1:G:138:LEU:CG	1:M:765:MET:HE2	2.44	0.48
2:P:41:LYS:HD2	3:U:733:ARG:NH2	2.29	0.48
3:U:720:LEU:O	3:U:724:ILE:HG12	2.14	0.48
2:Z:120:MET:HE1	2:Z:164:ALA:HB1	1.96	0.48
1:C:356:THR:HG21	1:C:546:VAL:HG12	1.96	0.48
3:F:733:ARG:HD2	2:R:41:LYS:HD2	120.96	0.48
1:W:768:GLU:CD	1:W:768:GLU:H	2.17	0.48
1:C:768:GLU:H	1:C:768:GLU:CD	2.19	0.47
1:G:206:ILE:HD11	1:G:394:PHE:HE1	5.54	0.47
1:G:768:GLU:CD	1:G:768:GLU:H	2.19	0.47
2:J:120:MET:HB2	2:J:168:ILE:HD12	1.95	0.47
3:F:717:ARG:NH2	3:U:728:GLU:HB3	2.29	0.47
2:X:31:PHE:O	2:X:51:ARG:NH1	2.46	0.47
3:F:720:LEU:O	3:F:724:ILE:HG13	2.15	0.47
2:H:120:MET:HE1	2:H:164:ALA:HB1	1.95	0.47
1:S:768:GLU:H	1:S:768:GLU:CD	2.17	0.47
1:A:611:SER:HB2	1:A:613:LEU:CD2	2.44	0.47
2:D:120:MET:HE3	2:D:164:ALA:HB1	2.96	0.47
1:O:766:THR:HG22	1:O:769:GLN:HG3	1.97	0.47
1:Q:611:SER:HB2	1:Q:613:LEU:CD2	2.44	0.47
1:S:518:LEU:HG	1:S:519:LYS:H	1.78	0.47
2:T:91:TYR:HB2	2:T:98:THR:HG23	1.95	0.47
1:Y:611:SER:HB2	1:Y:613:LEU:CD2	2.43	0.47
2:D:31:PHE:O	2:D:51:ARG:NH1	2.45	0.47
2:H:120:MET:HB2	2:H:168:ILE:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:206:ILE:HD11	1:Q:394:PHE:HE2	1.79	0.47
2:R:120:MET:HE1	2:R:164:ALA:HB1	1.96	0.47
2:Z:120:MET:HB2	2:Z:168:ILE:HD12	1.96	0.47
3:F:717:ARG:NH2	3:U:725:GLN:HA	2.29	0.47
1:A:324:LEU:O	1:A:333:LYS:HE3	2.15	0.47
1:I:138:LEU:HG	1:Q:769:GLN:CB	2.37	0.47
2:J:31:PHE:O	2:J:51:ARG:NH1	2.46	0.47
2:Z:91:TYR:HB2	2:Z:98:THR:HG23	1.95	0.47
1:O:518:LEU:HG	1:O:519:LYS:H	1.80	0.47
2:P:120:MET:HB2	2:P:168:ILE:HD12	1.96	0.47
1:Q:768:GLU:CD	1:Q:768:GLU:H	2.17	0.47
1:W:518:LEU:HG	1:W:519:LYS:H	1.80	0.47
1:G:324:LEU:O	1:G:333:LYS:HE3	2.15	0.47
1:G:178:GLN:CD	1:G:739:MET:CE	2.83	0.47
1:C:331:GLU:HB3	1:I:332:GLN:HE22	1.79	0.47
3:V:720:LEU:O	3:V:724:ILE:HG13	2.15	0.47
1:G:765:MET:HE2	1:M:138:LEU:HD11	1.97	0.47
1:Q:195:LYS:HB3	1:Q:196:PRO:HD3	1.97	0.47
1:Q:602:VAL:HG23	1:Q:607:VAL:CG2	2.45	0.47
1:C:178:GLN:CA	1:C:739:MET:HE1	2.44	0.47
1:M:611:SER:HB2	1:M:613:LEU:CD2	2.44	0.47
1:Q:329:THR:HG23	1:Q:332:GLN:H	1.80	0.47
3:F:728:GLU:HG2	3:U:717:ARG:HH21	1.80	0.47
2:B:80:TYR:CZ	3:E:746:MET:CE	2.99	0.46
1:G:363:VAL:HA	1:G:388:VAL:HG12	1.99	0.46
1:O:206:ILE:HD11	1:O:394:PHE:HE2	1.79	0.46
2:R:120:MET:HB2	2:R:168:ILE:HD12	1.97	0.46
2:T:120:MET:HE1	2:T:164:ALA:HB1	1.97	0.46
1:C:324:LEU:O	1:C:333:LYS:HE3	2.16	0.46
1:C:766:THR:HG22	1:C:769:GLN:HG3	1.98	0.46
2:N:120:MET:HB2	2:N:168:ILE:HD12	1.96	0.46
2:T:120:MET:HB2	2:T:168:ILE:HD12	1.97	0.46
1:S:602:VAL:HG23	1:S:607:VAL:CG2	2.45	0.46
1:Y:178:GLN:CD	1:Y:739:MET:CE	2.84	0.46
1:A:182:MET:HA	1:A:186:MET:HG3	1.98	0.46
1:M:324:LEU:O	1:M:333:LYS:HE3	2.15	0.46
1:O:324:LEU:O	1:O:333:LYS:HE3	2.15	0.46
2:P:31:PHE:O	2:P:51:ARG:NH1	2.45	0.46
1:Y:324:LEU:O	1:Y:333:LYS:HE3	2.15	0.46
1:A:195:LYS:HB3	1:A:196:PRO:HD3	1.98	0.46
3:E:717:ARG:NH1	3:V:724:ILE:HB	2.31	0.46
1:G:766:THR:HG22	1:G:769:GLN:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:766:THR:HG22	1:I:769:GLN:HG3	1.98	0.46
1:M:404:PRO:O	1:M:405:GLU:CB	2.64	0.46
1:W:324:LEU:O	1:W:333:LYS:HE3	2.16	0.46
1:A:176:LEU:N	1:A:177:PRO:CD	2.78	0.46
2:D:99:TYR:O	2:D:102:VAL:HG22	2.16	0.46
1:G:518:LEU:HG	1:G:519:LYS:N	2.32	0.46
1:O:178:GLN:CD	1:O:739:MET:CE	2.83	0.46
2:P:99:TYR:O	2:P:102:VAL:HG22	2.16	0.46
1:Q:518:LEU:HG	1:Q:519:LYS:H	1.79	0.46
2:X:120:MET:HB2	2:X:168:ILE:HD12	1.96	0.46
1:C:133:LEU:O	1:C:136:SER:OG	2.21	0.46
1:C:178:GLN:CD	1:C:739:MET:CE	2.84	0.46
1:C:182:MET:HA	1:C:186:MET:HG3	1.97	0.46
1:C:602:VAL:HG23	1:C:607:VAL:CG2	2.46	0.46
1:G:138:LEU:HD21	1:M:765:MET:SD	2.53	0.46
2:H:80:TYR:HE1	3:K:746:MET:SD	2.39	0.46
2:J:120:MET:HE1	2:J:164:ALA:HB1	1.97	0.46
2:N:99:TYR:O	2:N:102:VAL:HG22	2.16	0.46
1:S:329:THR:HG23	1:S:332:GLN:H	1.81	0.46
1:Y:133:LEU:O	1:Y:136:SER:OG	2.21	0.46
1:Y:768:GLU:H	1:Y:768:GLU:CD	2.18	0.46
2:H:176:VAL:HG23	2:H:177:SER:N	2.31	0.46
3:F:725:GLN:CA	3:K:717:ARG:NH2	122.10	0.46
1:M:182:MET:HA	1:M:186:MET:HG3	1.98	0.46
1:O:404:PRO:O	1:O:405:GLU:CB	2.64	0.46
1:O:611:SER:HB2	1:O:613:LEU:CD2	2.45	0.46
1:S:182:MET:HA	1:S:186:MET:HG3	1.98	0.46
1:S:206:ILE:HD11	1:S:394:PHE:HE2	1.80	0.46
1:W:182:MET:HA	1:W:186:MET:HG3	1.98	0.46
1:Y:182:MET:HA	1:Y:186:MET:HG3	1.98	0.46
2:B:99:TYR:O	2:B:102:VAL:HG22	2.16	0.46
2:H:99:TYR:O	2:H:102:VAL:HG22	2.16	0.46
1:I:133:LEU:O	1:I:136:SER:OG	2.21	0.46
2:B:176:VAL:HG23	2:B:177:SER:N	2.31	0.46
3:E:724:ILE:HG22	3:V:717:ARG:NE	2.31	0.46
1:G:195:LYS:HB3	1:G:196:PRO:HD3	1.98	0.46
1:M:766:THR:HG22	1:M:769:GLN:HG3	1.98	0.46
1:A:518:LEU:HG	1:A:519:LYS:H	1.81	0.45
2:B:80:TYR:OH	3:E:746:MET:CE	2.64	0.45
3:E:724:ILE:CG2	3:V:717:ARG:NE	2.78	0.45
2:N:31:PHE:O	2:N:51:ARG:NH1	2.46	0.45
1:Q:178:GLN:CD	1:Q:739:MET:CE	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:120:MET:HE1	2:D:164:ALA:HB1	1.98	0.45
2:B:80:TYR:CZ	3:E:746:MET:SD	3.09	0.45
2:J:99:TYR:O	2:J:102:VAL:HG22	2.17	0.45
1:M:329:THR:HG23	1:M:332:GLN:H	1.81	0.45
1:Q:324:LEU:O	1:Q:333:LYS:HE3	2.17	0.45
3:F:728:GLU:CG	3:U:717:ARG:NH2	2.78	0.45
1:A:363:VAL:HA	1:A:388:VAL:HG12	1.98	0.45
1:I:178:GLN:CD	1:I:739:MET:CE	2.84	0.45
1:M:588:ILE:HD12	1:M:593:GLY:HA2	1.98	0.45
1:O:195:LYS:HB3	1:O:196:PRO:HD3	1.97	0.45
1:O:518:LEU:HG	1:O:519:LYS:N	2.32	0.45
1:Q:363:VAL:HA	1:Q:388:VAL:HG12	1.98	0.45
1:Q:178:GLN:CA	1:Q:739:MET:HE1	2.44	0.45
1:C:138:LEU:CD2	1:S:769:GLN:OE1	2.61	0.45
1:Y:602:VAL:HG23	1:Y:607:VAL:CG2	2.47	0.45
1:I:404:PRO:O	1:I:405:GLU:CB	2.65	0.45
1:I:768:GLU:H	1:I:768:GLU:CD	2.19	0.45
2:J:79:ALA:HB2	3:L:746:MET:HE1	1.94	0.45
1:O:329:THR:HG23	1:O:332:GLN:H	1.81	0.45
3:F:728:GLU:HG2	3:U:717:ARG:NH2	2.31	0.45
1:A:178:GLN:CA	1:A:739:MET:HE1	2.43	0.45
1:C:404:PRO:O	1:C:405:GLU:CB	2.65	0.45
1:I:182:MET:HA	1:I:186:MET:HG3	1.97	0.45
1:Q:404:PRO:O	1:Q:405:GLU:CB	2.64	0.45
1:S:195:LYS:HB3	1:S:196:PRO:HD3	1.99	0.45
1:S:518:LEU:HG	1:S:519:LYS:N	2.31	0.45
1:W:602:VAL:HG23	1:W:607:VAL:CG2	2.46	0.45
2:X:99:TYR:O	2:X:102:VAL:HG22	2.16	0.45
1:C:195:LYS:HB3	1:C:196:PRO:HD3	1.99	0.45
1:I:206:ILE:HD11	1:I:394:PHE:CE2	2.51	0.45
1:I:607:VAL:O	1:I:611:SER:OG	2.20	0.45
2:R:38:LEU:HA	5:R:2000:GSP:O2'	2.16	0.45
2:R:99:TYR:O	2:R:102:VAL:HG22	2.16	0.45
1:S:404:PRO:O	1:S:405:GLU:CB	2.64	0.45
2:X:120:MET:HE3	2:X:164:ALA:HB1	1.97	0.45
2:Z:38:LEU:HA	5:Z:2000:GSP:O2'	2.16	0.45
1:A:768:GLU:CD	1:A:768:GLU:H	2.18	0.45
2:B:80:TYR:CE1	3:E:746:MET:CE	2.98	0.45
1:C:206:ILE:HD11	1:C:394:PHE:CE2	2.51	0.45
3:F:724:ILE:CG2	3:K:717:ARG:HD2	118.99	0.45
2:D:80:TYR:HE1	3:F:746:MET:HG2	1.82	0.45
1:G:602:VAL:HG23	1:G:607:VAL:CG2	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:602:VAL:HG23	1:I:607:VAL:CG2	2.47	0.45
1:M:602:VAL:HG23	1:M:607:VAL:CG2	2.46	0.45
1:S:324:LEU:O	1:S:333:LYS:HE3	2.17	0.45
1:S:178:GLN:CA	1:S:739:MET:HE1	2.44	0.45
1:Y:363:VAL:HA	1:Y:388:VAL:HG12	1.99	0.45
1:G:404:PRO:O	1:G:405:GLU:CB	2.65	0.45
1:G:178:GLN:CA	1:G:739:MET:HE1	2.46	0.45
1:O:588:ILE:HD12	1:O:593:GLY:HA2	1.99	0.45
1:Q:588:ILE:HD12	1:Q:593:GLY:HA2	1.98	0.45
1:W:404:PRO:O	1:W:405:GLU:CB	2.65	0.45
1:G:329:THR:HG23	1:G:332:GLN:H	1.82	0.45
1:I:329:THR:HG23	1:I:332:GLN:H	1.82	0.45
1:I:518:LEU:HG	1:I:519:LYS:N	2.31	0.45
1:M:176:LEU:N	1:M:177:PRO:CD	2.80	0.45
1:M:363:VAL:HA	1:M:388:VAL:HG12	1.99	0.45
1:Q:182:MET:HA	1:Q:186:MET:HG3	1.99	0.45
1:Q:196:PRO:HG2	2:R:131:LEU:HD22	1.98	0.45
2:T:99:TYR:O	2:T:102:VAL:HG22	2.16	0.45
1:A:329:THR:HG23	1:A:332:GLN:H	1.82	0.45
1:C:363:VAL:HA	1:C:388:VAL:HG12	2.01	0.45
1:C:518:LEU:HG	1:C:519:LYS:N	2.31	0.45
1:Y:588:ILE:HD12	1:Y:593:GLY:HA2	1.99	0.45
1:Y:766:THR:HG22	1:Y:769:GLN:HG3	1.99	0.45
2:D:38:LEU:CA	5:D:2000:GSP:O2'	2.86	0.44
1:S:363:VAL:HA	1:S:388:VAL:HG12	1.99	0.44
1:S:405:GLU:HA	1:S:534:PRO:HG3	1.99	0.44
3:E:717:ARG:HG2	3:V:728:GLU:OE2	2.12	0.44
1:Y:195:LYS:HB3	1:Y:196:PRO:HD3	1.99	0.44
1:Y:518:LEU:HG	1:Y:519:LYS:H	1.83	0.44
1:M:178:GLN:CA	1:M:739:MET:HE1	2.44	0.44
1:O:178:GLN:CA	1:O:739:MET:HE1	2.44	0.44
1:A:766:THR:HG22	1:A:769:GLN:HG3	2.00	0.44
1:C:588:ILE:HD12	1:C:593:GLY:HA2	1.98	0.44
1:I:324:LEU:O	1:I:333:LYS:HE3	2.16	0.44
1:M:195:LYS:HB3	1:M:196:PRO:HD3	1.98	0.44
1:O:602:VAL:HG23	1:O:607:VAL:CG2	2.47	0.44
1:Q:518:LEU:HG	1:Q:519:LYS:N	2.31	0.44
1:W:178:GLN:CD	1:W:739:MET:CE	2.85	0.44
1:A:336:ARG:HA	1:Y:537:HIS:CD2	2.53	0.44
1:G:176:LEU:N	1:G:177:PRO:CD	2.80	0.44
1:I:195:LYS:HB3	1:I:196:PRO:HD3	1.99	0.44
2:T:125:LYS:HG2	5:T:2000:GSP:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:518:LEU:HG	1:W:519:LYS:N	2.32	0.44
1:A:206:ILE:HD11	1:A:394:PHE:HE1	1.81	0.44
1:C:176:LEU:N	1:C:177:PRO:CD	2.81	0.44
1:G:206:ILE:HD11	1:G:394:PHE:HE2	1.81	0.44
1:I:759:GLU:OE2	1:Q:147:TYR:OH	2.33	0.44
2:R:26:ASN:ND2	5:R:2000:GSP:O1A	2.50	0.44
1:W:607:VAL:O	1:W:611:SER:OG	2.20	0.44
2:Z:99:TYR:O	2:Z:102:VAL:HG22	2.17	0.44
2:B:44:ILE:HD12	3:F:737:TYR:CE2	2.51	0.44
1:C:329:THR:HG23	1:C:332:GLN:H	1.83	0.44
2:H:104:ARG:HD2	2:H:104:ARG:HA	1.79	0.44
3:K:740:ARG:HH22	1:Q:682:SER:HB3	1.83	0.44
1:S:178:GLN:CD	1:S:739:MET:CE	2.85	0.44
3:F:733:ARG:CZ	2:R:41:LYS:HB3	122.00	0.44
2:T:176:VAL:HG23	2:T:177:SER:N	2.33	0.44
1:W:178:GLN:CA	1:W:739:MET:HE1	2.44	0.44
1:W:766:THR:HG22	1:W:769:GLN:HG3	1.98	0.44
1:Y:329:THR:HG23	1:Y:332:GLN:H	1.83	0.44
1:Y:404:PRO:O	1:Y:405:GLU:CB	2.65	0.44
1:I:588:ILE:HD12	1:I:593:GLY:HA2	1.98	0.44
3:F:717:ARG:HH11	3:K:728:GLU:HB2	123.26	0.44
3:K:738:ILE:HD11	3:L:738:ILE:HD13	1.99	0.44
1:Y:178:GLN:CA	1:Y:739:MET:HE1	2.45	0.44
1:A:588:ILE:HD12	1:A:593:GLY:HA2	1.99	0.44
2:B:26:ASN:ND2	5:B:2000:GSP:O1A	2.48	0.44
1:C:206:ILE:HD11	1:C:394:PHE:CE1	4.76	0.44
3:E:735:GLN:HE22	3:F:734:LEU:CD1	3.85	0.44
1:M:206:ILE:HD11	1:M:394:PHE:CE2	2.53	0.44
1:O:363:VAL:HA	1:O:388:VAL:HG12	2.00	0.44
1:A:178:GLN:CD	1:A:739:MET:HE3	2.39	0.43
1:A:404:PRO:O	1:A:405:GLU:CB	2.65	0.43
1:G:588:ILE:HD12	1:G:593:GLY:HA2	1.99	0.43
1:O:169:ASN:OD1	1:O:201:ARG:CZ	2.66	0.43
2:R:176:VAL:HG23	2:R:177:SER:N	2.34	0.43
1:W:176:LEU:N	1:W:177:PRO:CD	2.81	0.43
1:W:363:VAL:HA	1:W:388:VAL:HG12	2.00	0.43
1:C:571:TRP:CE2	1:C:578:LEU:HD12	2.55	0.43
1:I:405:GLU:HA	1:I:534:PRO:HG3	2.00	0.43
2:R:104:ARG:HD2	2:R:104:ARG:HA	1.79	0.43
2:B:80:TYR:CZ	3:E:746:MET:HE1	2.53	0.43
1:C:405:GLU:HA	1:C:534:PRO:HG3	2.00	0.43
3:E:752:ILE:HD13	3:F:745:ILE:CD1	4.40	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:40:SER:HB3	5:J:2000:GSP:H3'	2.00	0.43
1:A:571:TRP:CE2	1:A:578:LEU:HD12	2.53	0.43
1:C:331:GLU:HG3	1:I:332:GLN:NE2	2.32	0.43
2:N:104:ARG:HD2	2:N:104:ARG:HA	1.77	0.43
1:Y:518:LEU:HG	1:Y:519:LYS:N	2.34	0.43
1:I:221:SER:C	2:N:71:GLU:OE2	2.56	0.43
3:F:731:ASN:ND2	3:U:717:ARG:NH2	2.64	0.43
1:Y:206:ILE:HD11	1:Y:394:PHE:CE1	2.54	0.43
1:A:518:LEU:HG	1:A:519:LYS:N	2.33	0.43
1:O:176:LEU:N	1:O:177:PRO:CD	2.82	0.43
1:W:195:LYS:HB3	1:W:196:PRO:HD3	1.99	0.43
1:Y:176:LEU:N	1:Y:177:PRO:CD	2.81	0.43
1:G:206:ILE:HD11	1:G:394:PHE:CE1	4.79	0.43
1:C:138:LEU:HA	1:S:769:GLN:HE21	1.84	0.43
1:C:549:LYS:HD3	1:C:554:LEU:HD21	2.02	0.43
3:F:730:ILE:O	3:F:734:LEU:HG	2.20	0.43
1:M:169:ASN:OD1	1:M:201:ARG:CZ	2.67	0.43
1:O:405:GLU:HA	1:O:534:PRO:HG3	1.99	0.43
1:Q:206:ILE:HD11	1:Q:394:PHE:CE2	2.54	0.43
1:Q:405:GLU:HA	1:Q:534:PRO:HG3	2.01	0.43
1:W:588:ILE:HD12	1:W:593:GLY:HA2	1.99	0.43
2:P:176:VAL:HG23	2:P:177:SER:N	2.34	0.42
1:G:571:TRP:CE2	1:G:578:LEU:HD12	2.54	0.42
2:H:80:TYR:CE1	3:K:746:MET:SD	3.12	0.42
1:M:571:TRP:CE2	1:M:578:LEU:HD12	2.54	0.42
2:P:37:ASN:O	5:P:2000:GSP:O2'	2.21	0.42
1:Q:308:ALA:N	1:Q:309:PRO:CD	2.81	0.42
1:W:329:THR:HG23	1:W:332:GLN:H	1.82	0.42
1:C:138:LEU:CD1	1:W:765:MET:HE2	145.12	0.42
1:A:602:VAL:HG23	1:A:607:VAL:CG2	2.48	0.42
2:D:125:LYS:HG2	5:D:2000:GSP:C6	2.55	0.42
1:I:363:VAL:HA	1:I:388:VAL:HG12	2.01	0.42
3:V:730:ILE:O	3:V:734:LEU:HG	2.20	0.42
2:D:40:SER:HB3	5:D:2000:GSP:C3'	2.82	0.42
3:F:717:ARG:NH2	3:U:728:GLU:CB	2.82	0.42
1:I:176:LEU:N	1:I:177:PRO:CD	2.82	0.42
3:E:728:GLU:HB3	3:L:717:ARG:CZ	123.85	0.42
1:O:182:MET:HA	1:O:186:MET:HG3	2.02	0.42
1:I:138:LEU:CG	1:Q:769:GLN:HB3	2.49	0.42
1:W:206:ILE:HD11	1:W:394:PHE:CE2	2.53	0.42
3:E:730:ILE:O	3:E:734:LEU:HG	2.20	0.42
1:I:571:TRP:CE2	1:I:578:LEU:HD12	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:405:GLU:HA	1:M:534:PRO:HG3	2.00	0.42
2:N:176:VAL:HG23	2:N:177:SER:N	2.34	0.42
2:X:176:VAL:HG23	2:X:177:SER:N	2.34	0.42
1:S:206:ILE:HD11	1:S:394:PHE:CE2	2.55	0.42
2:H:80:TYR:CE1	3:K:746:MET:HE1	2.54	0.42
1:O:206:ILE:HD11	1:O:394:PHE:CE2	2.54	0.42
1:C:657:ARG:NH2	1:C:674:ASP:O	2.57	0.42
3:E:728:GLU:HB3	3:L:717:ARG:NH2	123.54	0.42
2:D:176:VAL:HG23	2:D:177:SER:N	2.36	0.42
1:Y:405:GLU:HA	1:Y:534:PRO:HG3	2.02	0.42
1:A:206:ILE:HD11	1:A:394:PHE:CE1	2.55	0.42
3:E:754:GLU:HA	2:R:48:PHE:HD2	125.19	0.42
3:K:730:ILE:O	3:K:734:LEU:HG	2.20	0.42
1:Q:176:LEU:N	1:Q:177:PRO:CD	2.83	0.42
1:Y:571:TRP:CE2	1:Y:578:LEU:HD12	2.55	0.42
2:Z:173:TYR:O	2:Z:173:TYR:CG	2.73	0.42
1:G:549:LYS:HD3	1:G:554:LEU:HD21	2.03	0.41
1:S:169:ASN:OD1	1:S:201:ARG:CZ	2.68	0.41
1:W:405:GLU:HA	1:W:534:PRO:HG3	2.02	0.41
1:W:196:PRO:HG2	2:X:131:LEU:HD22	2.02	0.41
2:B:173:TYR:CG	2:B:173:TYR:O	2.72	0.41
1:C:571:TRP:CD2	1:C:578:LEU:HD12	2.56	0.41
3:F:724:ILE:HA	3:F:727:GLN:HE21	1.85	0.41
1:I:169:ASN:OD1	1:I:201:ARG:CZ	2.68	0.41
2:J:173:TYR:CG	2:J:173:TYR:O	2.73	0.41
1:S:176:LEU:N	1:S:177:PRO:CD	2.83	0.41
2:P:41:LYS:HB3	3:U:733:ARG:HH22	1.83	0.41
1:G:169:ASN:OD1	1:G:201:ARG:CZ	2.68	0.41
2:H:80:TYR:OH	3:K:746:MET:HB3	2.19	0.41
1:M:308:ALA:N	1:M:309:PRO:CD	2.83	0.41
2:B:44:ILE:HD13	3:F:737:TYR:CD1	2.56	0.41
1:G:405:GLU:HA	1:G:534:PRO:HG3	2.02	0.41
2:P:104:ARG:HA	2:P:104:ARG:HD2	1.79	0.41
1:A:308:ALA:N	1:A:309:PRO:CD	2.83	0.41
1:C:169:ASN:OD1	1:C:201:ARG:CZ	2.68	0.41
1:G:206:ILE:HD11	1:G:394:PHE:CE2	2.55	0.41
1:W:169:ASN:OD1	1:W:201:ARG:CZ	2.68	0.41
1:A:571:TRP:CD2	1:A:578:LEU:HD12	2.56	0.41
3:E:731:ASN:HD21	3:F:731:ASN:CB	4.72	0.41
1:I:549:LYS:HD3	1:I:554:LEU:HD21	2.02	0.41
2:H:80:TYR:CE1	3:K:746:MET:CE	3.04	0.41
1:Q:169:ASN:OD1	1:Q:201:ARG:CZ	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Z:31:PHE:O	2:Z:51:ARG:NH1	2.46	0.41
1:C:332:GLN:NE2	1:I:332:GLN:HG3	2.30	0.41
3:V:724:ILE:HA	3:V:727:GLN:HE21	1.85	0.41
1:A:336:ARG:HE	1:Y:537:HIS:CE1	2.37	0.41
1:G:695:LEU:HD12	1:G:695:LEU:HA	1.97	0.41
2:H:31:PHE:O	2:H:51:ARG:NH1	2.46	0.41
1:S:549:LYS:HD3	1:S:554:LEU:HD21	2.02	0.41
1:S:578:LEU:CD2	1:S:717:LEU:HB3	2.51	0.41
1:Y:549:LYS:HD3	1:Y:554:LEU:HD21	2.02	0.41
1:Y:578:LEU:CD2	1:Y:717:LEU:HB3	2.50	0.41
1:A:196:PRO:HG2	2:B:131:LEU:HD22	2.01	0.41
2:B:31:PHE:O	2:B:51:ARG:NH1	2.46	0.41
1:O:571:TRP:CE2	1:O:578:LEU:HD12	2.56	0.41
1:Q:571:TRP:CE2	1:Q:578:LEU:HD12	2.55	0.41
1:S:766:THR:O	1:S:769:GLN:HB2	2.21	0.41
1:W:308:ALA:N	1:W:309:PRO:CD	2.84	0.41
1:Y:695:LEU:HA	1:Y:695:LEU:HD12	1.96	0.41
3:L:730:ILE:O	3:L:734:LEU:HG	2.19	0.41
1:C:332:GLN:HG3	1:I:332:GLN:HE21	1.85	0.41
1:I:133:LEU:HD11	1:I:138:LEU:HD22	2.03	0.41
1:Q:578:LEU:CD2	1:Q:717:LEU:HB3	2.52	0.41
3:U:730:ILE:O	3:U:734:LEU:HG	2.21	0.41
1:W:571:TRP:CE2	1:W:578:LEU:HD12	2.56	0.41
1:W:783:ARG:O	1:W:784:SER:CB	2.69	0.41
1:Y:657:ARG:NH2	1:Y:674:ASP:O	2.54	0.41
1:C:639:VAL:HG13	1:C:714:TYR:HB2	2.04	0.40
1:C:783:ARG:O	1:C:784:SER:CB	2.70	0.40
1:I:621:GLN:NE2	1:I:622:GLU:OE2	2.53	0.40
1:O:578:LEU:HD21	1:O:717:LEU:HB3	2.03	0.40
1:O:639:VAL:HG13	1:O:714:TYR:HB2	2.03	0.40
1:Q:549:LYS:HD3	1:Q:554:LEU:HD21	2.03	0.40
1:G:571:TRP:CD2	1:G:578:LEU:HD12	2.57	0.40
2:H:173:TYR:O	2:H:173:TYR:CG	2.73	0.40
1:M:571:TRP:CD2	1:M:578:LEU:HD12	2.55	0.40
1:M:783:ARG:O	1:M:784:SER:CB	2.70	0.40
1:O:783:ARG:O	1:O:784:SER:CB	2.69	0.40
1:S:571:TRP:CE2	1:S:578:LEU:HD12	2.55	0.40
2:T:173:TYR:O	2:T:173:TYR:CG	2.74	0.40
2:T:48:PHE:HD2	3:U:754:GLU:HA	1.86	0.40
1:W:549:LYS:HD3	1:W:554:LEU:HD21	2.03	0.40
2:X:104:ARG:HD2	2:X:104:ARG:HA	1.78	0.40
1:Y:783:ARG:O	1:Y:784:SER:CB	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:79:ALA:HB2	3:F:746:MET:HE1	2.01	0.40
1:G:783:ARG:O	1:G:784:SER:CB	2.70	0.40
1:Q:766:THR:O	1:Q:769:GLN:HB2	2.22	0.40
1:S:783:ARG:O	1:S:784:SER:CB	2.69	0.40
3:K:742:ILE:HD11	3:L:741:ILE:HD13	2.04	0.40
3:L:724:ILE:HA	3:L:727:GLN:HE21	1.86	0.40
1:O:578:LEU:CD2	1:O:717:LEU:HB3	2.51	0.40
1:W:657:ARG:NH2	1:W:674:ASP:O	2.54	0.40
1:Y:169:ASN:OD1	1:Y:201:ARG:CZ	2.69	0.40
1:C:133:LEU:HD11	1:C:138:LEU:HD22	2.04	0.40
1:I:139:PHE:HD1	1:I:143:MET:CE	2.34	0.40

All (61) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:174:ARG:NH2	1:M:166:CYS:O[2_545]	0.72	1.48
2:D:174:ARG:NH2	1:O:166:CYS:O[2_556]	0.76	1.44
2:B:174:ARG:NH2	1:g:166:CYS:O[2_656]	0.78	1.42
1:I:396:THR:OG1	1:M:627:THR:OG1[2_545]	0.85	1.35
1:C:396:THR:OG1	1:O:627:THR:OG1[2_556]	1.08	1.12
2:H:174:ARG:NH2	1:W:166:CYS:O[2_655]	1.08	1.12
1:S:346:HIS:O	1:Y:626:TYR:CE1[2_656]	1.08	1.12
1:S:346:HIS:CA	1:Y:626:TYR:OH[2_656]	1.20	1.00
1:Q:343:LEU:O	1:c:626:TYR:OH[2_655]	1.29	0.91
1:O:779:ASP:OD2	1:g:537:HIS:CD2[2_656]	1.37	0.83
2:D:174:ARG:CZ	1:O:166:CYS:O[2_556]	1.41	0.79
2:J:56:ASP:OD1	1:M:165:PHE:O[2_545]	1.44	0.76
2:B:56:ASP:OD1	1:g:165:PHE:O[2_656]	1.47	0.73
2:D:56:ASP:OD1	1:O:165:PHE:O[2_556]	1.47	0.73
2:J:174:ARG:CZ	1:M:166:CYS:O[2_545]	1.51	0.69
1:A:626:TYR:CD2	1:O:346:HIS:O[2_546]	1.53	0.67
1:G:626:TYR:OH	1:M:348:LEU:N[2_555]	1.55	0.65
1:G:626:TYR:CD2	1:M:346:HIS:O[2_555]	1.56	0.64
1:S:346:HIS:C	1:Y:626:TYR:OH[2_656]	1.61	0.59
1:S:346:HIS:O	1:Y:626:TYR:CZ[2_656]	1.61	0.59
1:A:626:TYR:OH	1:O:348:LEU:N[2_546]	1.63	0.57
1:G:626:TYR:CE2	1:M:346:HIS:O[2_555]	1.69	0.51
1:A:626:TYR:OH	1:O:348:LEU:O[2_546]	1.72	0.48
1:S:346:HIS:CA	1:Y:626:TYR:CZ[2_656]	1.75	0.45
1:A:626:TYR:CE2	1:O:346:HIS:O[2_546]	1.76	0.44
1:G:626:TYR:OH	1:M:348:LEU:O[2_555]	1.80	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:396:THR:OG1	1:g:627:THR:OG1[2_656]	1.81	0.39
1:S:323:ARG:NH1	1:Y:707:ASP:OD2[2_656]	1.81	0.39
2:B:174:ARG:CZ	1:g:166:CYS:O[2_656]	1.84	0.36
1:Q:346:HIS:CB	1:c:626:TYR:CZ[2_655]	1.84	0.36
2:B:174:ARG:NH2	1:g:166:CYS:C[2_656]	1.87	0.33
2:H:56:ASP:OD1	1:W:165:PHE:O[2_655]	1.87	0.33
1:I:396:THR:CB	1:M:627:THR:OG1[2_545]	1.87	0.33
2:H:174:ARG:CZ	1:W:166:CYS:O[2_655]	1.88	0.32
1:S:346:HIS:C	1:Y:626:TYR:CZ[2_656]	1.88	0.32
2:B:56:ASP:OD2	1:g:166:CYS:CA[2_656]	1.89	0.31
2:J:174:ARG:NH2	1:M:166:CYS:C[2_545]	1.93	0.27
1:G:339:SER:OG	1:c:537:HIS:CG[1_565]	1.94	0.26
2:D:174:ARG:NH2	1:O:166:CYS:C[2_556]	1.97	0.23
1:S:346:HIS:O	1:Y:626:TYR:OH[2_656]	1.98	0.22
1:S:346:HIS:CB	1:Y:626:TYR:CE2[2_656]	2.00	0.20
2:B:56:ASP:CG	1:g:166:CYS:CA[2_656]	2.01	0.19
1:A:616:LEU:CD2	1:O:346:HIS:CD2[2_546]	2.03	0.17
1:Q:346:HIS:CB	1:c:626:TYR:OH[2_655]	2.03	0.17
1:G:616:LEU:CD2	1:M:346:HIS:CD2[2_555]	2.07	0.13
1:S:346:HIS:C	1:Y:626:TYR:CE1[2_656]	2.07	0.13
1:C:396:THR:CB	1:O:627:THR:OG1[2_556]	2.08	0.12
2:B:56:ASP:O	2:h:130:HIS:CE1[2_656]	2.09	0.11
1:Q:323:ARG:NH1	1:c:707:ASP:OD2[2_655]	2.09	0.11
2:B:56:ASP:OD1	1:g:166:CYS:CA[2_656]	2.10	0.10
2:B:56:ASP:OD1	1:g:166:CYS:C[2_656]	2.10	0.10
1:G:326:THR:O	1:c:404:PRO:CD[1_565]	2.10	0.10
1:O:779:ASP:OD2	1:g:537:HIS:NE2[2_656]	2.10	0.10
1:G:396:THR:OG1	1:W:627:THR:OG1[2_655]	2.11	0.09
1:O:779:ASP:CG	1:g:537:HIS:CD2[2_656]	2.14	0.06
1:O:779:ASP:OD2	1:g:537:HIS:CG[2_656]	2.15	0.05
1:S:346:HIS:CB	1:Y:626:TYR:CZ[2_656]	2.17	0.03
1:A:626:TYR:CG	1:O:346:HIS:O[2_546]	2.18	0.02
1:S:346:HIS:N	1:Y:626:TYR:OH[2_656]	2.18	0.02
1:A:626:TYR:OH	1:O:348:LEU:C[2_546]	2.19	0.01
1:G:626:TYR:OH	1:M:348:LEU:CA[2_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	A	460/566 (81%)	442 (96%)	16 (4%)	2 (0%)	43	90
1	C	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	G	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	I	460/566 (81%)	440 (96%)	17 (4%)	3 (1%)	30	84
1	M	460/566 (81%)	441 (96%)	16 (4%)	3 (1%)	30	84
1	O	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	30	84
1	Q	460/566 (81%)	439 (95%)	19 (4%)	2 (0%)	43	90
1	S	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	W	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	30	84
1	Y	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	c	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	43	90
1	g	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	43	90
2	B	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	D	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	H	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	J	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	N	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	P	171/219 (78%)	162 (95%)	8 (5%)	1 (1%)	33	85
2	R	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	T	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	19	77
2	X	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	Z	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	19	77
2	d	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	h	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
3	E	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	F	30/48 (62%)	30 (100%)	0	0	100	100
3	K	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	L	30/48 (62%)	30 (100%)	0	0	100	100
3	U	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	V	30/48 (62%)	30 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	b	30/48 (62%)	30 (100%)	0	0	100	100
3	e	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	f	30/48 (62%)	30 (100%)	0	0	100	100
3	i	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	j	30/48 (62%)	30 (100%)	0	0	100	100
All	All	7986/9996 (80%)	7645 (96%)	295 (4%)	46 (1%)	33	85

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
2	B	68	ALA
1	C	405	GLU
2	D	68	ALA
1	G	405	GLU
2	H	68	ALA
1	I	405	GLU
2	J	68	ALA
1	M	405	GLU
2	N	68	ALA
1	O	405	GLU
2	P	68	ALA
1	Q	405	GLU
2	R	68	ALA
1	S	405	GLU
2	T	68	ALA
1	W	405	GLU
2	X	68	ALA
1	Y	405	GLU
2	Z	68	ALA
1	c	405	GLU
2	d	68	ALA
1	g	405	GLU
2	h	68	ALA
1	W	398	SER
1	C	398	SER
1	G	398	SER
1	I	398	SER
1	M	398	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	398	SER
1	S	398	SER
2	T	125	LYS
1	Y	398	SER
2	Z	125	LYS
1	A	399	VAL
1	O	399	VAL
1	W	399	VAL
1	g	399	VAL
1	C	399	VAL
1	G	399	VAL
1	I	399	VAL
1	M	399	VAL
1	Q	399	VAL
1	Y	399	VAL
1	c	399	VAL
1	S	399	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	C	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	G	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	I	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	M	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	O	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	Q	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	S	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	W	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	Y	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	c	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	g	422/508 (83%)	409 (97%)	13 (3%)	52	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	D	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	H	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	J	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	N	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	P	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	R	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	T	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	X	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	Z	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	d	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	h	147/191 (77%)	144 (98%)	3 (2%)	68	92
3	E	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	F	21/45 (47%)	21 (100%)	0	100	100
3	K	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	L	21/45 (47%)	21 (100%)	0	100	100
3	U	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	V	21/45 (47%)	21 (100%)	0	100	100
3	a	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	b	21/45 (47%)	21 (100%)	0	100	100
3	e	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	f	21/45 (47%)	21 (100%)	0	100	100
3	i	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	j	21/45 (47%)	21 (100%)	0	100	100
All	All	7140/8928 (80%)	6931 (97%)	209 (3%)	55	88

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

Mol	Chain	Res	Type
1	A	138	LEU
1	A	148	LEU
1	A	235	LYS
1	A	306	ARG
1	A	318	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	ARG
1	A	335	GLN
1	A	378	ASP
1	A	391	CYS
1	A	397	THR
1	A	565	LYS
1	A	613	LEU
1	A	694	LYS
1	A	739	MET
2	B	7	GLU
2	B	33	ARG
2	B	54	GLN
1	C	138	LEU
1	C	148	LEU
1	C	235	LYS
1	C	306	ARG
1	C	318	MET
1	C	323	ARG
1	C	335	GLN
1	C	378	ASP
1	C	391	CYS
1	C	397	THR
1	C	565	LYS
1	C	613	LEU
1	C	694	LYS
1	C	739	MET
2	D	7	GLU
2	D	33	ARG
2	D	54	GLN
3	E	728	GLU
1	G	138	LEU
1	G	148	LEU
1	G	235	LYS
1	G	306	ARG
1	G	318	MET
1	G	323	ARG
1	G	335	GLN
1	G	378	ASP
1	G	391	CYS
1	G	397	THR
1	G	565	LYS
1	G	613	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	694	LYS
1	G	739	MET
2	H	7	GLU
2	H	33	ARG
2	H	54	GLN
1	I	138	LEU
1	I	148	LEU
1	I	235	LYS
1	I	306	ARG
1	I	318	MET
1	I	323	ARG
1	I	335	GLN
1	I	378	ASP
1	I	391	CYS
1	I	397	THR
1	I	565	LYS
1	I	613	LEU
1	I	694	LYS
1	I	739	MET
2	J	7	GLU
2	J	33	ARG
2	J	54	GLN
3	K	728	GLU
1	M	138	LEU
1	M	148	LEU
1	M	235	LYS
1	M	306	ARG
1	M	318	MET
1	M	323	ARG
1	M	335	GLN
1	M	378	ASP
1	M	391	CYS
1	M	397	THR
1	M	565	LYS
1	M	613	LEU
1	M	694	LYS
1	M	739	MET
2	N	7	GLU
2	N	33	ARG
2	N	54	GLN
1	O	138	LEU
1	O	148	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	235	LYS
1	O	306	ARG
1	O	318	MET
1	O	323	ARG
1	O	335	GLN
1	O	378	ASP
1	O	391	CYS
1	O	397	THR
1	O	565	LYS
1	O	613	LEU
1	O	694	LYS
1	O	739	MET
2	P	7	GLU
2	P	33	ARG
2	P	54	GLN
1	Q	138	LEU
1	Q	148	LEU
1	Q	235	LYS
1	Q	306	ARG
1	Q	318	MET
1	Q	323	ARG
1	Q	335	GLN
1	Q	378	ASP
1	Q	391	CYS
1	Q	397	THR
1	Q	565	LYS
1	Q	613	LEU
1	Q	694	LYS
1	Q	739	MET
2	R	7	GLU
2	R	33	ARG
2	R	54	GLN
1	S	138	LEU
1	S	148	LEU
1	S	235	LYS
1	S	306	ARG
1	S	318	MET
1	S	323	ARG
1	S	335	GLN
1	S	378	ASP
1	S	391	CYS
1	S	397	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	565	LYS
1	S	613	LEU
1	S	694	LYS
1	S	739	MET
2	T	7	GLU
2	T	33	ARG
2	T	54	GLN
3	U	728	GLU
1	W	138	LEU
1	W	148	LEU
1	W	235	LYS
1	W	306	ARG
1	W	318	MET
1	W	323	ARG
1	W	335	GLN
1	W	378	ASP
1	W	391	CYS
1	W	397	THR
1	W	565	LYS
1	W	613	LEU
1	W	694	LYS
1	W	739	MET
2	X	7	GLU
2	X	33	ARG
2	X	54	GLN
1	Y	138	LEU
1	Y	148	LEU
1	Y	235	LYS
1	Y	306	ARG
1	Y	318	MET
1	Y	323	ARG
1	Y	335	GLN
1	Y	378	ASP
1	Y	391	CYS
1	Y	397	THR
1	Y	565	LYS
1	Y	613	LEU
1	Y	694	LYS
1	Y	739	MET
2	Z	7	GLU
2	Z	33	ARG
2	Z	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	a	728	GLU
1	c	138	LEU
1	c	148	LEU
1	c	235	LYS
1	c	306	ARG
1	c	318	MET
1	c	323	ARG
1	c	335	GLN
1	c	378	ASP
1	c	391	CYS
1	c	397	THR
1	c	565	LYS
1	c	613	LEU
1	c	694	LYS
1	c	739	MET
2	d	7	GLU
2	d	33	ARG
2	d	54	GLN
3	e	728	GLU
1	g	138	LEU
1	g	148	LEU
1	g	235	LYS
1	g	306	ARG
1	g	318	MET
1	g	323	ARG
1	g	378	ASP
1	g	391	CYS
1	g	397	THR
1	g	565	LYS
1	g	613	LEU
1	g	694	LYS
1	g	739	MET
2	h	7	GLU
2	h	33	ARG
2	h	54	GLN
3	i	728	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	540	ASN
1	A	606	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	332	GLN
1	C	540	ASN
1	C	606	GLN
3	F	727	GLN
3	F	731	ASN
1	G	540	ASN
1	G	606	GLN
1	I	332	GLN
1	I	540	ASN
1	I	606	GLN
1	I	776	GLN
3	K	731	ASN
3	K	735	GLN
3	L	727	GLN
3	L	731	ASN
1	M	540	ASN
1	M	606	GLN
1	O	393	ASN
1	O	540	ASN
1	O	606	GLN
1	Q	540	ASN
1	Q	606	GLN
1	S	393	ASN
1	S	540	ASN
1	S	606	GLN
3	U	731	ASN
3	U	735	GLN
3	V	727	GLN
1	W	540	ASN
1	W	606	GLN
1	W	776	GLN
1	Y	540	ASN
1	Y	606	GLN
3	b	727	GLN
1	c	540	ASN
1	c	606	GLN
3	e	731	ASN
3	e	735	GLN
3	f	727	GLN
1	g	540	ASN
1	g	606	GLN
1	g	776	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	i	735	GLN
3	j	727	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	093	A	2002	-	25,25,25	4.21	9 (36%)	33,36,36	4.60	17 (51%)
5	GSP	B	2000	6	34,34,34	1.54	7 (20%)	52,54,54	4.94	13 (25%)
4	093	C	2002	-	25,25,25	4.23	9 (36%)	33,36,36	4.57	17 (51%)
5	GSP	D	2000	6	34,34,34	1.62	8 (23%)	52,54,54	3.98	16 (30%)
4	093	G	2002	1	25,25,25	4.21	9 (36%)	33,36,36	4.59	17 (51%)
5	GSP	H	2000	6	34,34,34	1.42	7 (20%)	52,54,54	4.39	13 (25%)
4	093	I	2002	-	25,25,25	4.23	9 (36%)	33,36,36	4.57	17 (51%)
5	GSP	J	2000	6	34,34,34	1.68	8 (23%)	52,54,54	4.34	15 (28%)
4	093	M	2002	-	25,25,25	4.22	9 (36%)	33,36,36	4.60	17 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GSP	N	2000	6	34,34,34	1.50	7 (20%)	52,54,54	4.20	17 (32%)
4	093	O	2002	1	25,25,25	4.23	9 (36%)	33,36,36	4.62	17 (51%)
5	GSP	P	2000	6	34,34,34	1.49	8 (23%)	52,54,54	3.96	15 (28%)
4	093	Q	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.59	17 (51%)
5	GSP	R	2000	6	34,34,34	1.43	7 (20%)	52,54,54	3.34	13 (25%)
4	093	S	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.62	17 (51%)
5	GSP	T	2000	6	34,34,34	1.34	7 (20%)	52,54,54	4.00	15 (28%)
4	093	W	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.62	17 (51%)
5	GSP	X	2000	6	34,34,34	1.51	9 (26%)	52,54,54	3.76	15 (28%)
4	093	Y	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.60	17 (51%)
5	GSP	Z	2000	6	34,34,34	1.52	8 (23%)	52,54,54	4.02	16 (30%)
4	093	c	2002	1	25,25,25	4.23	9 (36%)	33,36,36	4.64	17 (51%)
5	GSP	d	2000	6	34,34,34	1.53	8 (23%)	52,54,54	4.60	14 (26%)
4	093	g	2002	1	25,25,25	4.23	9 (36%)	33,36,36	4.59	17 (51%)
5	GSP	h	2000	6	34,34,34	1.57	10 (29%)	52,54,54	4.01	15 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	093	A	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	B	2000	6	-	0/21/38/38	0/3/3/3
4	093	C	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	D	2000	6	-	0/21/38/38	0/3/3/3
4	093	G	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	H	2000	6	-	0/21/38/38	0/3/3/3
4	093	I	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	J	2000	6	-	0/21/38/38	0/3/3/3
4	093	M	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	N	2000	6	-	0/21/38/38	0/3/3/3
4	093	O	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	P	2000	6	-	0/21/38/38	0/3/3/3
4	093	Q	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	R	2000	6	-	0/21/38/38	0/3/3/3
4	093	S	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	T	2000	6	-	0/21/38/38	0/3/3/3
4	093	W	2002	1	-	0/17/19/19	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GSP	X	2000	6	-	0/21/38/38	0/3/3/3
4	093	Y	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	Z	2000	6	-	0/21/38/38	0/3/3/3
4	093	c	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	d	2000	6	-	0/21/38/38	0/3/3/3
4	093	g	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	h	2000	6	-	0/21/38/38	0/3/3/3

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2002	093	CAI-SAP	-15.42	1.55	1.75
4	Y	2002	093	CAI-SAP	-15.37	1.55	1.75
4	O	2002	093	CAI-SAP	-15.34	1.55	1.75
4	g	2002	093	CAI-SAP	-15.34	1.55	1.75
4	c	2002	093	CAI-SAP	-15.33	1.55	1.75
4	S	2002	093	CAI-SAP	-15.32	1.55	1.75
4	I	2002	093	CAI-SAP	-15.32	1.55	1.75
4	W	2002	093	CAI-SAP	-15.30	1.55	1.75
4	A	2002	093	CAI-SAP	-15.29	1.55	1.75
4	M	2002	093	CAI-SAP	-15.28	1.55	1.75
4	Q	2002	093	CAI-SAP	-15.28	1.55	1.75
4	G	2002	093	CAI-SAP	-15.28	1.55	1.75
4	I	2002	093	CAQ-SAP	-8.29	1.59	1.73
4	Q	2002	093	CAQ-SAP	-8.28	1.59	1.73
4	S	2002	093	CAQ-SAP	-8.25	1.59	1.73
4	A	2002	093	CAQ-SAP	-8.25	1.59	1.73
4	W	2002	093	CAQ-SAP	-8.24	1.59	1.73
4	M	2002	093	CAQ-SAP	-8.23	1.59	1.73
4	O	2002	093	CAQ-SAP	-8.23	1.59	1.73
4	c	2002	093	CAQ-SAP	-8.23	1.59	1.73
4	g	2002	093	CAQ-SAP	-8.22	1.59	1.73
4	C	2002	093	CAQ-SAP	-8.19	1.59	1.73
4	Y	2002	093	CAQ-SAP	-8.16	1.59	1.73
4	G	2002	093	CAQ-SAP	-8.16	1.59	1.73
4	W	2002	093	CAJ-NAK	7.31	1.47	1.38
4	G	2002	093	CAJ-NAK	7.31	1.47	1.38
4	I	2002	093	CAJ-NAK	7.29	1.47	1.38
4	g	2002	093	CAJ-NAK	7.29	1.47	1.38
4	S	2002	093	CAJ-NAK	7.26	1.47	1.38
4	Y	2002	093	CAJ-NAK	7.26	1.47	1.38
4	A	2002	093	CAJ-NAK	7.25	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	2002	093	CAJ-NAK	7.24	1.47	1.38
4	M	2002	093	CAJ-NAK	7.23	1.47	1.38
4	O	2002	093	CAJ-NAK	7.21	1.47	1.38
4	C	2002	093	CAJ-NAK	7.21	1.47	1.38
4	c	2002	093	CAJ-NAK	7.20	1.47	1.38
4	c	2002	093	SAN-NAU	4.91	1.67	1.61
4	G	2002	093	SAN-NAU	4.89	1.67	1.61
4	M	2002	093	SAN-NAU	4.89	1.67	1.61
4	Y	2002	093	SAN-NAU	4.89	1.67	1.61
4	O	2002	093	SAN-NAU	4.88	1.67	1.61
4	W	2002	093	SAN-NAU	4.88	1.67	1.61
4	Q	2002	093	SAN-NAU	4.87	1.67	1.61
4	C	2002	093	SAN-NAU	4.86	1.67	1.61
4	I	2002	093	SAN-NAU	4.82	1.67	1.61
4	S	2002	093	SAN-NAU	4.82	1.67	1.61
4	A	2002	093	SAN-NAU	4.80	1.67	1.61
4	g	2002	093	SAN-NAU	4.77	1.67	1.61
5	N	2000	GSP	C4-N9	-4.54	1.31	1.37
5	P	2000	GSP	C4-N9	-4.39	1.31	1.37
4	Q	2002	093	CAQ-NAR	4.24	1.45	1.32
4	S	2002	093	CAQ-NAR	4.23	1.45	1.32
4	W	2002	093	CAQ-NAR	4.23	1.45	1.32
4	O	2002	093	CAQ-NAR	4.22	1.45	1.32
4	g	2002	093	CAQ-NAR	4.21	1.45	1.32
4	M	2002	093	CAQ-NAR	4.21	1.45	1.32
4	c	2002	093	CAQ-NAR	4.21	1.45	1.32
4	G	2002	093	CAQ-NAR	4.20	1.45	1.32
4	Y	2002	093	CAQ-NAR	4.20	1.45	1.32
4	A	2002	093	CAQ-NAR	4.19	1.45	1.32
4	I	2002	093	CAQ-NAR	4.19	1.45	1.32
4	C	2002	093	CAQ-NAR	4.17	1.45	1.32
5	Z	2000	GSP	C4-N9	-3.95	1.32	1.37
5	d	2000	GSP	C4-N9	-3.94	1.32	1.37
5	h	2000	GSP	O4'-C1'	3.72	1.45	1.41
5	J	2000	GSP	C4-N9	-3.70	1.32	1.37
5	X	2000	GSP	O4'-C1'	3.48	1.45	1.41
5	D	2000	GSP	C5-C4	3.40	1.48	1.40
5	J	2000	GSP	PG-S1G	3.35	1.97	1.90
5	J	2000	GSP	C5-C4	3.35	1.48	1.40
5	B	2000	GSP	PG-S1G	3.30	1.97	1.90
5	R	2000	GSP	C5-C4	3.20	1.47	1.40
4	c	2002	093	OAM-SAN	-3.17	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2000	GSP	C2-N3	3.16	1.37	1.33
5	T	2000	GSP	C5-C4	3.15	1.47	1.40
4	O	2002	093	OAM-SAN	-3.13	1.40	1.43
4	M	2002	093	OAM-SAN	-3.12	1.40	1.43
5	B	2000	GSP	C4-N9	-3.12	1.33	1.37
5	h	2000	GSP	C5-C4	3.11	1.47	1.40
4	g	2002	093	OAM-SAN	-3.10	1.40	1.43
5	D	2000	GSP	PG-S1G	3.08	1.96	1.90
4	W	2002	093	OAM-SAN	-3.08	1.40	1.43
4	G	2002	093	CAS-NAR	3.05	1.44	1.38
4	C	2002	093	OAM-SAN	-3.05	1.40	1.43
4	S	2002	093	OAM-SAN	-3.04	1.40	1.43
4	A	2002	093	OAM-SAN	-3.04	1.40	1.43
5	h	2000	GSP	PG-S1G	3.03	1.96	1.90
4	C	2002	093	CAS-NAR	3.03	1.44	1.38
4	M	2002	093	CAS-NAR	3.02	1.44	1.38
4	Q	2002	093	OAM-SAN	-3.03	1.40	1.43
4	c	2002	093	CAS-NAR	3.02	1.44	1.38
5	Z	2000	GSP	C5-C4	3.00	1.47	1.40
5	X	2000	GSP	C5-C4	3.00	1.47	1.40
5	B	2000	GSP	PG-O2G	3.00	1.65	1.55
4	O	2002	093	CAS-NAR	2.99	1.44	1.38
4	I	2002	093	OAM-SAN	-2.99	1.40	1.43
4	G	2002	093	OAM-SAN	-2.98	1.40	1.43
4	A	2002	093	CAS-NAR	2.98	1.44	1.38
5	d	2000	GSP	C5-C4	2.97	1.47	1.40
4	I	2002	093	CAS-NAR	2.97	1.44	1.38
4	S	2002	093	CAS-NAR	2.96	1.44	1.38
4	Y	2002	093	OAM-SAN	-2.96	1.40	1.43
4	g	2002	093	CAS-NAR	2.96	1.44	1.38
4	Q	2002	093	CAS-NAR	2.95	1.44	1.38
5	J	2000	GSP	C5-N7	-2.95	1.34	1.38
5	B	2000	GSP	C5-C4	2.95	1.47	1.40
5	J	2000	GSP	C2-N2	2.95	1.36	1.32
4	W	2002	093	CAS-NAR	2.95	1.44	1.38
4	Y	2002	093	CAS-NAR	2.94	1.44	1.38
5	B	2000	GSP	C6-N1	-2.92	1.32	1.36
5	Z	2000	GSP	PG-O2G	2.91	1.65	1.55
5	P	2000	GSP	PG-S1G	2.91	1.96	1.90
5	D	2000	GSP	C4-N9	-2.89	1.33	1.37
5	H	2000	GSP	C5-C4	2.87	1.47	1.40
5	J	2000	GSP	C2-N3	2.87	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	2000	GSP	C2-N3	2.87	1.37	1.33
4	Y	2002	093	CAT-CAS	2.86	1.53	1.49
4	I	2002	093	CAT-CAS	2.86	1.53	1.49
4	C	2002	093	CAT-CAS	2.84	1.53	1.49
5	T	2000	GSP	C4-N9	-2.83	1.33	1.37
5	J	2000	GSP	PG-O2G	2.81	1.65	1.55
5	h	2000	GSP	PG-O2G	2.80	1.65	1.55
4	O	2002	093	CAT-CAS	2.80	1.53	1.49
4	Q	2002	093	CAT-CAS	2.80	1.53	1.49
5	d	2000	GSP	PG-O2G	2.78	1.64	1.55
4	M	2002	093	CAT-CAS	2.77	1.53	1.49
4	g	2002	093	CAT-CAS	2.77	1.53	1.49
4	A	2002	093	CAT-CAS	2.77	1.53	1.49
5	H	2000	GSP	C4-N9	-2.77	1.33	1.37
4	G	2002	093	CAT-CAS	2.75	1.53	1.49
5	D	2000	GSP	C2-N2	2.73	1.36	1.32
5	N	2000	GSP	PG-O2G	2.73	1.64	1.55
4	W	2002	093	CAT-CAS	2.72	1.53	1.49
4	c	2002	093	CAT-CAS	2.72	1.53	1.49
4	S	2002	093	CAT-CAS	2.71	1.53	1.49
5	X	2000	GSP	C4-N9	-2.68	1.33	1.37
5	R	2000	GSP	PG-O2G	2.67	1.64	1.55
5	B	2000	GSP	C5-N7	-2.63	1.35	1.38
5	N	2000	GSP	C5-N7	-2.62	1.35	1.38
5	H	2000	GSP	PG-O2G	2.61	1.64	1.55
5	D	2000	GSP	C5-N7	-2.59	1.35	1.38
5	D	2000	GSP	PG-O2G	2.55	1.64	1.55
5	d	2000	GSP	PG-S1G	2.55	1.95	1.90
5	R	2000	GSP	C4-N9	-2.53	1.34	1.37
5	P	2000	GSP	C5-C4	2.50	1.46	1.40
5	N	2000	GSP	C5-C4	2.49	1.46	1.40
5	H	2000	GSP	C6-N1	-2.49	1.33	1.36
5	Z	2000	GSP	PG-S1G	2.48	1.95	1.90
5	Z	2000	GSP	C5-N7	-2.48	1.35	1.38
5	X	2000	GSP	C2-N3	2.43	1.36	1.33
5	P	2000	GSP	PG-O2G	2.42	1.63	1.55
5	H	2000	GSP	PG-S1G	2.40	1.95	1.90
5	H	2000	GSP	C5-N7	-2.37	1.35	1.38
5	T	2000	GSP	C5-N7	-2.37	1.35	1.38
5	N	2000	GSP	PG-S1G	2.36	1.95	1.90
5	d	2000	GSP	C2-N2	2.36	1.35	1.32
5	h	2000	GSP	C2-N3	2.35	1.36	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	2000	GSP	C6-N1	-2.35	1.33	1.36
5	X	2000	GSP	C5-N7	-2.34	1.35	1.38
5	T	2000	GSP	C2-N3	2.34	1.36	1.33
5	H	2000	GSP	C2-N3	2.32	1.36	1.33
5	h	2000	GSP	C2-N2	2.32	1.35	1.32
5	d	2000	GSP	C5-N7	-2.32	1.35	1.38
5	R	2000	GSP	PG-S1G	2.30	1.95	1.90
5	R	2000	GSP	C5-N7	-2.30	1.35	1.38
4	I	2002	093	CAV-CAW	-2.29	1.41	1.50
4	G	2002	093	CAV-CAW	-2.28	1.42	1.50
5	d	2000	GSP	C2-N3	2.28	1.36	1.33
4	Y	2002	093	CAV-CAW	-2.28	1.42	1.50
4	C	2002	093	CAV-CAW	-2.28	1.42	1.50
4	g	2002	093	CAV-CAW	-2.28	1.42	1.50
5	h	2000	GSP	C5-N7	-2.27	1.35	1.38
4	S	2002	093	CAV-CAW	-2.27	1.42	1.50
4	Q	2002	093	CAV-CAW	-2.27	1.42	1.50
4	W	2002	093	CAV-CAW	-2.27	1.42	1.50
5	X	2000	GSP	PG-S1G	2.27	1.95	1.90
5	P	2000	GSP	C2-N3	2.27	1.36	1.33
4	c	2002	093	CAV-CAW	-2.27	1.42	1.50
5	T	2000	GSP	C6-N1	-2.26	1.33	1.36
4	M	2002	093	CAV-CAW	-2.25	1.42	1.50
4	A	2002	093	CAV-CAW	-2.25	1.42	1.50
4	O	2002	093	CAV-CAW	-2.24	1.42	1.50
5	B	2000	GSP	C2-N3	2.23	1.36	1.33
5	d	2000	GSP	PG-O3G	2.23	1.63	1.55
5	X	2000	GSP	C6-N1	-2.23	1.33	1.36
5	X	2000	GSP	PG-O2G	2.22	1.62	1.55
5	P	2000	GSP	C5-N7	-2.21	1.35	1.38
5	T	2000	GSP	O4'-C1'	2.20	1.44	1.41
5	D	2000	GSP	O4'-C1'	2.20	1.44	1.41
5	Z	2000	GSP	O4'-C1'	2.19	1.44	1.41
5	T	2000	GSP	PG-O2G	2.17	1.62	1.55
5	h	2000	GSP	C6-N1	-2.17	1.33	1.36
5	R	2000	GSP	C2-N2	2.15	1.35	1.32
5	P	2000	GSP	PG-O3G	2.13	1.62	1.55
5	N	2000	GSP	C2-N3	2.10	1.36	1.33
5	X	2000	GSP	C2-N2	2.09	1.35	1.32
5	h	2000	GSP	C4-N9	-2.09	1.34	1.37
5	Z	2000	GSP	C2-N3	2.07	1.36	1.33
5	Z	2000	GSP	C6-N1	-2.06	1.33	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	h	2000	GSP	PG-O3G	2.05	1.62	1.55
5	J	2000	GSP	O4'-C1'	2.01	1.43	1.41
5	N	2000	GSP	C6-N1	-2.01	1.33	1.36

All (381) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2000	GSP	C6-C5-N7	22.61	137.18	134.14
5	h	2000	GSP	C6-C5-N7	22.16	137.12	134.14
5	B	2000	GSP	O3B-PG-S1G	-22.11	104.72	114.53
5	d	2000	GSP	C6-C5-N7	21.28	137.01	134.14
5	d	2000	GSP	O3B-PG-S1G	-21.17	105.14	114.53
5	X	2000	GSP	C6-C5-N7	20.56	136.91	134.14
5	N	2000	GSP	O3B-PG-S1G	-20.47	105.45	114.53
5	H	2000	GSP	O3B-PG-S1G	-20.09	105.62	114.53
5	J	2000	GSP	C6-C5-N7	19.90	136.82	134.14
5	D	2000	GSP	C6-C5-N7	19.72	136.80	134.14
5	T	2000	GSP	O3B-PG-S1G	-19.39	105.92	114.53
5	Z	2000	GSP	O3B-PG-S1G	-19.09	106.06	114.53
4	S	2002	093	OAO-SAN-OAM	-18.98	94.51	119.55
4	g	2002	093	OAO-SAN-OAM	-18.96	94.53	119.55
4	Q	2002	093	OAO-SAN-OAM	-18.95	94.55	119.55
4	G	2002	093	OAO-SAN-OAM	-18.94	94.56	119.55
4	C	2002	093	OAO-SAN-OAM	-18.94	94.56	119.55
4	A	2002	093	OAO-SAN-OAM	-18.93	94.57	119.55
4	I	2002	093	OAO-SAN-OAM	-18.93	94.57	119.55
4	M	2002	093	OAO-SAN-OAM	-18.92	94.58	119.55
4	Y	2002	093	OAO-SAN-OAM	-18.92	94.58	119.55
4	W	2002	093	OAO-SAN-OAM	-18.92	94.59	119.55
4	O	2002	093	OAO-SAN-OAM	-18.91	94.60	119.55
4	c	2002	093	OAO-SAN-OAM	-18.90	94.61	119.55
5	J	2000	GSP	O3B-PG-S1G	-18.87	106.16	114.53
5	H	2000	GSP	C6-C5-N7	18.27	136.60	134.14
5	P	2000	GSP	C6-C5-N7	18.11	136.58	134.14
5	Z	2000	GSP	C6-C5-N7	16.35	136.34	134.14
5	P	2000	GSP	O3B-PG-S1G	-15.04	107.86	114.53
5	R	2000	GSP	O3B-PG-S1G	-14.94	107.90	114.53
5	N	2000	GSP	C6-C5-N7	14.67	136.12	134.14
5	D	2000	GSP	O3B-PG-S1G	-14.61	108.05	114.53
5	T	2000	GSP	C6-C5-N7	12.50	135.82	134.14
5	h	2000	GSP	O3B-PG-S1G	-9.85	110.16	114.53
5	R	2000	GSP	C6-C5-N7	9.74	135.45	134.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	2000	GSP	O3B-PG-S1G	-9.57	110.28	114.53
4	c	2002	093	CAQ-NAK-CAJ	-9.49	111.49	112.36
4	O	2002	093	CAQ-NAK-CAJ	-9.26	111.51	112.36
4	W	2002	093	CAQ-NAK-CAJ	-9.22	111.52	112.36
4	S	2002	093	CAQ-NAK-CAJ	-9.21	111.52	112.36
4	Y	2002	093	CAQ-NAK-CAJ	-9.04	111.53	112.36
5	T	2000	GSP	O3G-PG-S1G	-9.02	103.22	112.73
4	M	2002	093	CAQ-NAK-CAJ	-9.01	111.54	112.36
4	A	2002	093	CAQ-NAK-CAJ	-8.95	111.54	112.36
4	Q	2002	093	CAQ-NAK-CAJ	-8.87	111.55	112.36
4	g	2002	093	CAQ-NAK-CAJ	-8.81	111.55	112.36
4	G	2002	093	CAQ-NAK-CAJ	-8.76	111.56	112.36
4	I	2002	093	CAQ-NAK-CAJ	-8.57	111.58	112.36
4	C	2002	093	CAQ-NAK-CAJ	-8.43	111.59	112.36
5	N	2000	GSP	O3G-PG-S1G	-7.37	104.96	112.73
4	c	2002	093	CAE-CAJ-CAI	-7.22	125.62	131.22
4	Y	2002	093	CAE-CAJ-CAI	-7.21	125.63	131.22
4	A	2002	093	CAE-CAJ-CAI	-7.20	125.64	131.22
4	W	2002	093	CAE-CAJ-CAI	-7.20	125.64	131.22
4	G	2002	093	CAE-CAJ-CAI	-7.19	125.65	131.22
5	H	2000	GSP	C5-C4-N3	-7.18	117.80	126.07
4	M	2002	093	CAE-CAJ-CAI	-7.18	125.66	131.22
4	O	2002	093	CAE-CAJ-CAI	-7.17	125.66	131.22
4	C	2002	093	CAE-CAJ-CAI	-7.15	125.68	131.22
4	I	2002	093	CAE-CAJ-CAI	-7.12	125.70	131.22
5	h	2000	GSP	C5-C4-N3	-7.09	117.90	126.07
4	g	2002	093	CAE-CAJ-CAI	-7.09	125.72	131.22
4	Q	2002	093	CAE-CAJ-CAI	-7.09	125.73	131.22
4	S	2002	093	CAE-CAJ-CAI	-7.06	125.74	131.22
5	B	2000	GSP	C5-C4-N3	-7.05	117.94	126.07
5	P	2000	GSP	O3G-PG-S1G	-7.00	105.35	112.73
5	B	2000	GSP	O2G-PG-S1G	6.61	119.69	112.73
5	T	2000	GSP	C5-C4-N3	-6.52	118.56	126.07
5	X	2000	GSP	C5-C4-N3	-6.42	118.67	126.07
4	C	2002	093	CAT-CAS-NAR	6.38	121.00	114.80
4	G	2002	093	CAT-CAS-NAR	6.38	121.00	114.80
4	W	2002	093	CAT-CAS-NAR	6.36	120.98	114.80
4	A	2002	093	CAT-CAS-NAR	6.36	120.98	114.80
5	R	2000	GSP	O3G-PG-S1G	-6.36	106.03	112.73
4	I	2002	093	CAT-CAS-NAR	6.36	120.98	114.80
4	Y	2002	093	CAT-CAS-NAR	6.34	120.96	114.80
4	g	2002	093	CAT-CAS-NAR	6.32	120.95	114.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2002	093	CAT-CAS-NAR	6.32	120.94	114.80
4	c	2002	093	CAT-CAS-NAR	6.32	120.94	114.80
5	D	2000	GSP	C5-C4-N3	-6.31	118.80	126.07
4	Q	2002	093	CAT-CAS-NAR	6.29	120.91	114.80
4	M	2002	093	CAT-CAS-NAR	6.28	120.90	114.80
4	O	2002	093	CAT-CAS-NAR	6.28	120.90	114.80
5	R	2000	GSP	C5-C4-N3	-6.21	118.92	126.07
5	R	2000	GSP	N3-C4-N9	6.17	135.96	126.91
5	J	2000	GSP	C5-C4-N3	-5.97	119.19	126.07
5	H	2000	GSP	N3-C4-N9	5.87	135.52	126.91
5	h	2000	GSP	N3-C4-N9	5.71	135.29	126.91
5	Z	2000	GSP	C5-C4-N3	-5.57	119.65	126.07
5	T	2000	GSP	N3-C4-N9	5.53	135.02	126.91
5	d	2000	GSP	C5-C4-N3	-5.48	119.76	126.07
5	N	2000	GSP	C8-N9-C4	5.47	111.41	106.96
5	T	2000	GSP	PB-O3B-PG	-5.46	113.31	132.05
5	X	2000	GSP	N3-C4-N9	5.39	134.82	126.91
5	P	2000	GSP	C5-C4-N3	-5.31	119.96	126.07
5	h	2000	GSP	C2-N3-C4	5.29	121.65	115.30
5	H	2000	GSP	O3G-PG-S1G	-5.29	107.15	112.73
5	B	2000	GSP	N3-C4-N9	5.20	134.54	126.91
5	D	2000	GSP	N3-C4-N9	5.20	134.53	126.91
5	H	2000	GSP	PB-O3B-PG	-5.19	114.24	132.05
5	B	2000	GSP	O3G-PG-S1G	-5.16	107.29	112.73
5	N	2000	GSP	PB-O3B-PG	-5.15	114.37	132.05
5	h	2000	GSP	O3G-PG-S1G	-5.12	107.33	112.73
5	N	2000	GSP	N3-C4-N9	5.12	134.42	126.91
5	d	2000	GSP	PB-O3B-PG	-5.12	114.48	132.05
5	R	2000	GSP	PB-O3B-PG	-5.12	114.50	132.05
5	P	2000	GSP	N3-C4-N9	5.10	134.39	126.91
5	J	2000	GSP	PB-O3B-PG	-5.05	114.73	132.05
5	Z	2000	GSP	PB-O3B-PG	-4.99	114.93	132.05
5	Z	2000	GSP	N3-C4-N9	4.97	134.20	126.91
5	P	2000	GSP	C8-N9-C4	4.94	110.97	106.96
5	D	2000	GSP	PB-O3B-PG	-4.92	115.17	132.05
5	B	2000	GSP	PB-O3B-PG	-4.90	115.24	132.05
4	S	2002	093	OAO-SAN-NAU	4.84	115.18	107.06
4	Q	2002	093	OAO-SAN-NAU	4.82	115.15	107.06
4	Y	2002	093	OAO-SAN-NAU	4.82	115.15	107.06
4	O	2002	093	OAO-SAN-NAU	4.81	115.13	107.06
4	A	2002	093	OAO-SAN-NAU	4.81	115.12	107.06
4	W	2002	093	OAO-SAN-NAU	4.80	115.11	107.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2002	093	OAO-SAN-NAU	4.80	115.11	107.06
4	c	2002	093	OAO-SAN-NAU	4.79	115.10	107.06
5	X	2000	GSP	PB-O3B-PG	-4.79	115.60	132.05
4	g	2002	093	OAO-SAN-NAU	4.78	115.08	107.06
4	M	2002	093	OAO-SAN-NAU	4.78	115.08	107.06
4	I	2002	093	OAO-SAN-NAU	4.78	115.07	107.06
4	C	2002	093	OAO-SAN-NAU	4.78	115.07	107.06
5	P	2000	GSP	PB-O3B-PG	-4.75	115.73	132.05
5	N	2000	GSP	C5-C4-N3	-4.72	120.63	126.07
5	J	2000	GSP	C4-C5-N7	-4.64	104.93	109.41
5	H	2000	GSP	C2-N3-C4	4.63	120.85	115.30
5	d	2000	GSP	N3-C4-N9	4.60	133.66	126.91
5	h	2000	GSP	PB-O3B-PG	-4.58	116.34	132.05
5	J	2000	GSP	N3-C4-N9	4.52	133.53	126.91
5	Z	2000	GSP	O3G-PG-S1G	-4.51	107.98	112.73
5	X	2000	GSP	C2-N3-C4	4.49	120.68	115.30
5	B	2000	GSP	C2-N3-C4	4.47	120.67	115.30
5	X	2000	GSP	O3G-PG-S1G	-4.34	108.15	112.73
5	D	2000	GSP	C4-C5-N7	-4.33	105.22	109.41
4	g	2002	093	OAM-SAN-NAU	4.33	114.32	107.06
5	R	2000	GSP	C2-N3-C4	4.32	120.48	115.30
4	S	2002	093	OAM-SAN-NAU	4.31	114.28	107.06
4	Q	2002	093	OAM-SAN-NAU	4.30	114.27	107.06
5	B	2000	GSP	C4-C5-N7	-4.30	105.26	109.41
4	A	2002	093	OAM-SAN-NAU	4.29	114.26	107.06
4	I	2002	093	OAM-SAN-NAU	4.29	114.26	107.06
4	W	2002	093	OAM-SAN-NAU	4.29	114.25	107.06
4	c	2002	093	CAI-CAJ-NAK	4.28	108.76	106.87
4	G	2002	093	OAM-SAN-NAU	4.28	114.24	107.06
4	M	2002	093	OAM-SAN-NAU	4.27	114.21	107.06
4	c	2002	093	OAM-SAN-NAU	4.26	114.20	107.06
4	C	2002	093	OAM-SAN-NAU	4.26	114.20	107.06
4	A	2002	093	CAI-CAJ-NAK	4.26	108.75	106.87
5	N	2000	GSP	PA-O3A-PB	-4.25	120.16	131.93
4	Y	2002	093	OAM-SAN-NAU	4.25	114.18	107.06
4	O	2002	093	OAM-SAN-NAU	4.24	114.18	107.06
4	M	2002	093	CAI-CAJ-NAK	4.24	108.74	106.87
4	W	2002	093	CAI-CAJ-NAK	4.23	108.74	106.87
4	O	2002	093	CAI-CAJ-NAK	4.22	108.73	106.87
4	G	2002	093	CAI-CAJ-NAK	4.16	108.71	106.87
4	Y	2002	093	CAI-CAJ-NAK	4.09	108.67	106.87
4	S	2002	093	CAI-CAJ-NAK	4.09	108.67	106.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2000	GSP	PA-O3A-PB	-4.08	120.64	131.93
4	Q	2002	093	CAI-CAJ-NAK	4.06	108.66	106.87
5	B	2000	GSP	PA-O3A-PB	-4.05	120.71	131.93
5	d	2000	GSP	C2-N3-C4	4.04	120.14	115.30
4	C	2002	093	OAM-SAN-CAF	4.04	114.14	107.68
4	c	2002	093	OAM-SAN-CAF	4.03	114.13	107.68
4	g	2002	093	CAI-CAJ-NAK	4.02	108.64	106.87
4	M	2002	093	OAM-SAN-CAF	4.01	114.09	107.68
4	I	2002	093	OAM-SAN-CAF	4.00	114.08	107.68
5	D	2000	GSP	C2-N3-C4	4.00	120.10	115.30
4	Y	2002	093	OAM-SAN-CAF	3.99	114.07	107.68
4	G	2002	093	OAM-SAN-CAF	3.99	114.06	107.68
4	O	2002	093	OAO-SAN-CAF	3.98	114.05	107.68
4	S	2002	093	OAO-SAN-CAF	3.98	114.05	107.68
4	Q	2002	093	OAO-SAN-CAF	3.99	114.05	107.68
4	Y	2002	093	OAO-SAN-CAF	3.98	114.05	107.68
4	O	2002	093	OAM-SAN-CAF	3.98	114.05	107.68
4	C	2002	093	OAO-SAN-CAF	3.98	114.05	107.68
5	H	2000	GSP	C4-C5-N7	-3.98	105.57	109.41
4	W	2002	093	OAM-SAN-CAF	3.98	114.04	107.68
4	g	2002	093	OAM-SAN-CAF	3.98	114.04	107.68
4	M	2002	093	OAO-SAN-CAF	3.97	114.03	107.68
4	A	2002	093	OAM-SAN-CAF	3.97	114.03	107.68
5	R	2000	GSP	C6-N1-C2	3.97	122.44	120.20
4	W	2002	093	OAO-SAN-CAF	3.96	114.02	107.68
4	Q	2002	093	OAM-SAN-CAF	3.96	114.02	107.68
4	S	2002	093	OAM-SAN-CAF	3.96	114.01	107.68
4	G	2002	093	OAO-SAN-CAF	3.96	114.01	107.68
4	C	2002	093	CAI-CAJ-NAK	3.96	108.61	106.87
4	g	2002	093	OAO-SAN-CAF	3.95	114.00	107.68
4	I	2002	093	OAO-SAN-CAF	3.95	113.99	107.68
4	c	2002	093	OAO-SAN-CAF	3.94	113.98	107.68
4	I	2002	093	CAI-CAJ-NAK	3.94	108.61	106.87
4	A	2002	093	OAO-SAN-CAF	3.94	113.98	107.68
5	P	2000	GSP	PA-O3A-PB	-3.89	121.16	131.93
5	T	2000	GSP	C2-N3-C4	3.88	119.96	115.30
5	H	2000	GSP	O2G-PG-S1G	3.86	116.80	112.73
5	D	2000	GSP	PA-O3A-PB	-3.77	121.49	131.93
5	d	2000	GSP	PA-O3A-PB	-3.77	121.49	131.93
5	J	2000	GSP	O2G-PG-S1G	3.76	116.69	112.73
5	Z	2000	GSP	C8-N9-C4	3.68	109.95	106.96
5	R	2000	GSP	C8-N9-C4	3.68	109.95	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2000	GSP	O3G-PG-S1G	-3.64	108.89	112.73
5	R	2000	GSP	PA-O3A-PB	-3.63	121.87	131.93
5	J	2000	GSP	C2-N3-C4	3.61	119.64	115.30
5	X	2000	GSP	PA-O3A-PB	-3.61	121.92	131.93
5	h	2000	GSP	C4-C5-N7	-3.61	105.92	109.41
5	T	2000	GSP	PA-O3A-PB	-3.60	121.97	131.93
5	P	2000	GSP	O3A-PB-O3B	3.58	108.94	101.66
5	h	2000	GSP	PA-O3A-PB	-3.55	122.09	131.93
5	Z	2000	GSP	PA-O3A-PB	-3.49	122.25	131.93
5	J	2000	GSP	PA-O3A-PB	-3.49	122.28	131.93
5	R	2000	GSP	O3A-PA-O5'	-3.45	93.78	102.91
5	J	2000	GSP	C6-N1-C2	3.43	122.14	120.20
5	N	2000	GSP	O2G-PG-S1G	3.41	116.32	112.73
5	Z	2000	GSP	C2-N3-C4	3.37	119.34	115.30
5	P	2000	GSP	C2-N3-C4	3.31	119.27	115.30
5	Z	2000	GSP	C4-C5-N7	-3.30	106.22	109.41
4	g	2002	093	OAX-CAW-CAV	-3.22	99.44	111.69
4	A	2002	093	OAX-CAW-CAV	-3.22	99.45	111.69
4	G	2002	093	OAX-CAW-CAV	-3.22	99.46	111.69
4	W	2002	093	OAX-CAW-CAV	-3.21	99.47	111.69
4	c	2002	093	OAX-CAW-CAV	-3.21	99.47	111.69
4	O	2002	093	OAX-CAW-CAV	-3.21	99.49	111.69
4	Q	2002	093	OAX-CAW-CAV	-3.21	99.49	111.69
4	M	2002	093	OAX-CAW-CAV	-3.21	99.49	111.69
4	S	2002	093	OAX-CAW-CAV	-3.20	99.51	111.69
4	A	2002	093	CAH-CAI-SAP	3.20	122.57	116.31
4	C	2002	093	OAX-CAW-CAV	-3.20	99.52	111.69
4	Y	2002	093	OAX-CAW-CAV	-3.20	99.53	111.69
4	G	2002	093	CAH-CAI-SAP	3.19	122.54	116.31
4	I	2002	093	OAX-CAW-CAV	-3.18	99.60	111.69
4	W	2002	093	CAH-CAI-SAP	3.17	122.52	116.31
5	T	2000	GSP	C4-C5-N7	-3.17	106.35	109.41
5	X	2000	GSP	C4-C5-N7	-3.16	106.35	109.41
4	S	2002	093	CAH-CAI-SAP	3.16	122.48	116.31
4	I	2002	093	CAH-CAI-SAP	3.15	122.48	116.31
4	C	2002	093	CAH-CAI-SAP	3.15	122.47	116.31
4	M	2002	093	CAH-CAI-SAP	3.15	122.47	116.31
4	Y	2002	093	CAH-CAI-SAP	3.15	122.47	116.31
4	O	2002	093	CAH-CAI-SAP	3.14	122.46	116.31
5	d	2000	GSP	C8-N9-C4	3.14	109.51	106.96
4	Q	2002	093	CAH-CAI-SAP	3.13	122.44	116.31
5	N	2000	GSP	O3A-PB-O3B	3.12	108.01	101.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	2002	093	CAH-CAI-SAP	3.12	122.42	116.31
4	g	2002	093	CAH-CAI-SAP	3.12	122.41	116.31
5	N	2000	GSP	C6-N1-C2	3.09	121.94	120.20
5	D	2000	GSP	O3G-PG-S1G	-3.05	109.51	112.73
5	P	2000	GSP	C4-C5-N7	-3.04	106.47	109.41
5	d	2000	GSP	O3A-PB-O3B	3.02	107.81	101.66
5	d	2000	GSP	O3A-PA-O5'	-3.02	94.92	102.91
5	d	2000	GSP	C4-C5-N7	-3.00	106.51	109.41
5	X	2000	GSP	C2'-C3'-C4'	3.00	108.63	102.64
4	M	2002	093	CAD-CAH-CAG	2.99	122.25	118.19
4	c	2002	093	OAL-CAS-NAR	-2.98	118.23	123.61
4	G	2002	093	OAL-CAS-NAR	-2.97	118.25	123.61
4	S	2002	093	OAL-CAS-NAR	-2.97	118.25	123.61
4	c	2002	093	CAD-CAH-CAG	2.97	122.23	118.19
4	O	2002	093	OAL-CAS-NAR	-2.96	118.26	123.61
4	g	2002	093	CAD-CAH-CAG	2.96	122.22	118.19
4	C	2002	093	CAD-CAH-CAG	2.96	122.21	118.19
4	g	2002	093	OAL-CAS-NAR	-2.95	118.27	123.61
4	O	2002	093	CAD-CAH-CAG	2.95	122.21	118.19
4	C	2002	093	OAL-CAS-NAR	-2.95	118.28	123.61
4	A	2002	093	OAL-CAS-NAR	-2.95	118.28	123.61
4	W	2002	093	OAL-CAS-NAR	-2.95	118.29	123.61
4	Y	2002	093	CAD-CAH-CAG	2.95	122.20	118.19
5	T	2000	GSP	O3A-PB-O3B	2.95	107.66	101.66
4	I	2002	093	CAD-CAH-CAG	2.95	122.20	118.19
4	S	2002	093	CAD-CAH-CAG	2.94	122.19	118.19
4	I	2002	093	OAL-CAS-NAR	-2.94	118.30	123.61
4	M	2002	093	OAL-CAS-NAR	-2.94	118.30	123.61
4	W	2002	093	CAD-CAH-CAG	2.93	122.18	118.19
5	N	2000	GSP	C2-N3-C4	2.93	118.81	115.30
5	H	2000	GSP	C8-N9-C4	2.93	109.34	106.96
5	D	2000	GSP	C6-N1-C2	2.93	121.85	120.20
4	Q	2002	093	OAL-CAS-NAR	-2.92	118.33	123.61
4	Y	2002	093	OAL-CAS-NAR	-2.92	118.33	123.61
4	Q	2002	093	CAD-CAH-CAG	2.92	122.16	118.19
4	c	2002	093	CAD-CAH-CAI	-2.91	118.70	120.94
4	G	2002	093	CAD-CAH-CAG	2.90	122.14	118.19
4	M	2002	093	CAD-CAH-CAI	-2.90	118.71	120.94
4	A	2002	093	CAD-CAH-CAG	2.90	122.13	118.19
5	D	2000	GSP	C8-N9-C4	2.89	109.31	106.96
4	g	2002	093	CAD-CAH-CAI	-2.87	118.73	120.94
4	O	2002	093	CAD-CAH-CAI	-2.84	118.75	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2000	GSP	N2-C2-N3	-2.81	116.62	120.28
4	Q	2002	093	CAD-CAH-CAI	-2.81	118.78	120.94
5	X	2000	GSP	O3A-PB-O3B	2.79	107.33	101.66
4	S	2002	093	CAD-CAH-CAI	-2.79	118.80	120.94
4	C	2002	093	CAD-CAH-CAI	-2.79	118.80	120.94
5	D	2000	GSP	O3A-PA-O5'	-2.78	95.54	102.91
5	h	2000	GSP	C2'-C3'-C4'	2.78	108.19	102.64
4	I	2002	093	CAD-CAH-CAI	-2.77	118.81	120.94
4	W	2002	093	CAD-CAH-CAI	-2.75	118.82	120.94
5	P	2000	GSP	O2G-PG-S1G	2.74	115.62	112.73
5	H	2000	GSP	O3A-PA-O5'	-2.73	95.69	102.91
4	Y	2002	093	CAD-CAH-CAI	-2.72	118.85	120.94
4	G	2002	093	CAD-CAH-CAI	-2.69	118.87	120.94
5	T	2000	GSP	C6-N1-C2	2.69	121.72	120.20
4	Y	2002	093	CAG-CAH-CAI	-2.68	118.88	120.94
5	T	2000	GSP	O2G-PG-S1G	2.67	115.54	112.73
4	A	2002	093	CAD-CAH-CAI	-2.66	118.89	120.94
4	A	2002	093	CAG-CAH-CAI	-2.65	118.90	120.94
5	d	2000	GSP	C6-N1-C2	2.65	121.69	120.20
4	C	2002	093	CAG-CAH-CAI	-2.64	118.91	120.94
4	I	2002	093	CAG-CAH-CAI	-2.63	118.92	120.94
4	G	2002	093	CAG-CAH-CAI	-2.63	118.92	120.94
5	h	2000	GSP	O3A-PB-O3B	2.62	107.00	101.66
4	W	2002	093	CAG-CAH-CAI	-2.62	118.93	120.94
5	h	2000	GSP	O3G-PG-O2G	2.61	111.19	105.97
4	S	2002	093	CAG-CAH-CAI	-2.61	118.94	120.94
5	D	2000	GSP	N2-C2-N3	-2.60	116.90	120.28
4	C	2002	093	CAE-CAJ-NAK	2.60	125.70	122.64
5	N	2000	GSP	C4-C5-N7	-2.59	106.91	109.41
4	I	2002	093	CAE-CAJ-NAK	2.59	125.69	122.64
4	Y	2002	093	CAE-CAJ-NAK	2.59	125.69	122.64
5	Z	2000	GSP	O3G-PG-O2G	2.58	111.14	105.97
4	M	2002	093	CAG-CAH-CAI	-2.57	118.96	120.94
4	O	2002	093	CAG-CAH-CAI	-2.56	118.97	120.94
4	G	2002	093	CAE-CAJ-NAK	2.55	125.64	122.64
4	g	2002	093	CAG-CAH-CAI	-2.55	118.98	120.94
4	g	2002	093	CAE-CAJ-NAK	2.54	125.63	122.64
5	T	2000	GSP	C8-N9-C4	2.54	109.02	106.96
4	Q	2002	093	CAG-CAH-CAI	-2.53	118.99	120.94
4	W	2002	093	CAE-CAJ-NAK	2.53	125.62	122.64
4	c	2002	093	CAE-CAJ-NAK	2.53	125.62	122.64
4	A	2002	093	CAE-CAJ-NAK	2.53	125.62	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	2002	093	CAE-CAJ-NAK	2.52	125.61	122.64
4	c	2002	093	CAG-CAH-CAI	-2.52	119.00	120.94
4	M	2002	093	CAE-CAJ-NAK	2.52	125.61	122.64
4	O	2002	093	CAE-CAJ-NAK	2.52	125.60	122.64
4	S	2002	093	CAE-CAJ-NAK	2.50	125.58	122.64
5	J	2000	GSP	C8-N9-C4	2.46	108.96	106.96
5	X	2000	GSP	C8-N9-C4	2.45	108.95	106.96
5	h	2000	GSP	C6-N1-C2	2.45	121.58	120.20
5	B	2000	GSP	N2-C2-N3	-2.42	117.13	120.28
5	X	2000	GSP	O3G-PG-O2G	2.41	110.80	105.97
5	D	2000	GSP	O3A-PB-O3B	2.36	106.46	101.66
5	N	2000	GSP	C1'-N9-C4	-2.36	122.56	126.64
5	Z	2000	GSP	O3A-PB-O3B	2.35	106.45	101.66
5	N	2000	GSP	C4'-O4'-C1'	-2.32	107.17	109.72
5	R	2000	GSP	C4-C5-N7	-2.29	107.19	109.41
5	d	2000	GSP	C1'-N9-C4	-2.27	122.71	126.64
5	D	2000	GSP	C2'-C3'-C4'	2.27	107.17	102.64
5	Z	2000	GSP	C6-N1-C2	2.27	121.48	120.20
5	d	2000	GSP	C2'-C3'-C4'	2.26	107.15	102.64
5	P	2000	GSP	C1'-N9-C4	-2.26	122.73	126.64
5	J	2000	GSP	O3A-PA-O5'	-2.25	96.95	102.91
5	R	2000	GSP	O3A-PB-O3B	2.16	106.06	101.66
4	Q	2002	093	CAF-SAN-NAU	-2.16	105.07	107.79
5	T	2000	GSP	N2-C2-N3	-2.16	117.47	120.28
4	S	2002	093	CAF-SAN-NAU	-2.15	105.08	107.79
4	c	2002	093	CAF-SAN-NAU	-2.15	105.08	107.79
4	Y	2002	093	CAF-SAN-NAU	-2.15	105.08	107.79
5	B	2000	GSP	O3A-PA-O5'	-2.15	97.22	102.91
4	C	2002	093	CAF-SAN-NAU	-2.14	105.09	107.79
4	O	2002	093	CAF-SAN-NAU	-2.14	105.10	107.79
4	W	2002	093	CAF-SAN-NAU	-2.13	105.10	107.79
4	M	2002	093	CAF-SAN-NAU	-2.13	105.11	107.79
4	G	2002	093	CAF-SAN-NAU	-2.12	105.12	107.79
5	N	2000	GSP	O2B-PB-O1B	2.12	123.86	112.14
4	g	2002	093	CAF-SAN-NAU	-2.12	105.13	107.79
5	h	2000	GSP	C8-N9-C4	2.11	108.68	106.96
4	I	2002	093	CAF-SAN-NAU	-2.11	105.13	107.79
4	A	2002	093	CAF-SAN-NAU	-2.11	105.14	107.79
5	J	2000	GSP	O2B-PB-O1B	2.10	123.78	112.14
5	B	2000	GSP	N1-C2-N3	2.09	124.61	121.78
5	P	2000	GSP	O2B-PB-O1B	2.09	123.72	112.14
5	N	2000	GSP	O3G-PG-O2G	2.09	110.14	105.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	2000	GSP	N2-C2-N3	-2.08	117.57	120.28
5	X	2000	GSP	O2B-PB-O1B	2.08	123.67	112.14
5	Z	2000	GSP	C2'-C3'-C4'	2.08	106.79	102.64
5	D	2000	GSP	O2B-PB-O1B	2.08	123.64	112.14
5	T	2000	GSP	C2'-C3'-C4'	2.06	106.75	102.64
5	Z	2000	GSP	N1-C2-N3	2.05	124.55	121.78
5	h	2000	GSP	O2B-PB-O1B	2.05	123.50	112.14
5	H	2000	GSP	O3A-PB-O3B	2.04	105.81	101.66
5	P	2000	GSP	C6-N1-C2	2.03	121.35	120.20
5	X	2000	GSP	C6-N1-C2	2.00	121.33	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/566 (83%)	0.72	34 (7%) 15 21	95, 212, 331, 500	0
1	C	470/566 (83%)	1.09	85 (18%) 2 6	126, 300, 456, 500	0
1	G	470/566 (83%)	0.77	34 (7%) 15 21	98, 214, 342, 500	0
1	I	470/566 (83%)	1.24	95 (20%) 2 5	124, 306, 474, 500	0
1	M	470/566 (83%)	0.79	42 (8%) 10 18	95, 217, 341, 500	0
1	O	470/566 (83%)	0.76	40 (8%) 11 18	102, 208, 335, 500	0
1	Q	470/566 (83%)	0.99	67 (14%) 3 9	102, 247, 364, 498	0
1	S	470/566 (83%)	1.05	71 (15%) 3 8	114, 251, 389, 500	0
1	W	470/566 (83%)	0.86	62 (13%) 4 10	99, 253, 387, 500	0
1	Y	470/566 (83%)	0.76	40 (8%) 11 18	115, 250, 365, 474	0
1	c	470/566 (83%)	1.28	104 (22%) 1 5	119, 305, 478, 500	0
1	g	470/566 (83%)	0.99	77 (16%) 2 7	126, 268, 416, 500	0
2	B	173/219 (78%)	0.75	19 (10%) 6 13	94, 201, 375, 493	0
2	D	173/219 (78%)	0.87	22 (12%) 4 11	95, 220, 341, 488	0
2	H	173/219 (78%)	0.90	22 (12%) 4 11	94, 207, 382, 499	0
2	J	173/219 (78%)	0.84	12 (6%) 17 23	92, 198, 338, 500	0
2	N	173/219 (78%)	1.40	43 (24%) 1 5	137, 282, 424, 496	0
2	P	173/219 (78%)	1.30	48 (27%) 1 4	132, 277, 432, 496	0
2	R	173/219 (78%)	1.10	39 (22%) 1 5	139, 269, 415, 496	0
2	T	173/219 (78%)	0.81	25 (14%) 3 9	136, 266, 407, 493	0
2	X	173/219 (78%)	0.95	34 (19%) 2 6	146, 282, 453, 500	0
2	Z	173/219 (78%)	0.70	13 (7%) 14 21	165, 262, 362, 494	0
2	d	173/219 (78%)	0.83	27 (15%) 3 8	146, 308, 447, 500	0
2	h	173/219 (78%)	1.10	36 (20%) 1 5	158, 294, 440, 500	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	E	41/48 (85%)	0.71	2 (4%) 28 30	153, 251, 365, 489	0
3	F	32/48 (66%)	0.25	1 (3%) 47 41	169, 285, 399, 466	0
3	K	41/48 (85%)	0.78	2 (4%) 28 30	131, 240, 410, 465	0
3	L	32/48 (66%)	0.50	1 (3%) 47 41	170, 263, 384, 436	0
3	U	41/48 (85%)	0.92	7 (17%) 2 7	175, 284, 408, 494	0
3	V	32/48 (66%)	0.59	1 (3%) 47 41	170, 260, 403, 435	0
3	a	41/48 (85%)	1.17	9 (21%) 1 5	195, 318, 423, 476	0
3	b	32/48 (66%)	1.59	12 (37%) 1 3	213, 309, 428, 479	0
3	e	41/48 (85%)	0.61	1 (2%) 56 47	175, 255, 384, 478	0
3	f	32/48 (66%)	0.38	1 (3%) 47 41	194, 288, 337, 363	0
3	i	41/48 (85%)	1.20	11 (26%) 1 5	202, 325, 441, 500	0
3	j	32/48 (66%)	0.66	2 (6%) 19 25	194, 282, 404, 462	0
All	All	8154/9996 (81%)	0.94	1141 (13%) 3 9	92, 255, 416, 500	0

All (1141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	523	GLN	12.4
1	C	517	ALA	11.4
1	c	695	LEU	10.4
1	I	522	TRP	9.9
1	g	405	GLU	9.3
1	I	372	VAL	8.0
1	C	523	GLN	7.9
1	W	515	ALA	7.8
1	c	705	GLY	7.7
1	I	370	GLN	7.6
1	I	517	ALA	7.5
2	h	166	GLN	7.5
1	Y	695	LEU	7.4
2	Z	73	TYR	7.4
1	S	219	TYR	7.4
1	W	350	ALA	7.3
1	I	513	PRO	7.3
1	I	382	TYR	7.1
1	c	782	MET	7.1
1	g	404	PRO	7.0
2	N	50	THR	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	c	376	SER	6.8
1	c	706	LEU	6.7
2	Z	72	ARG	6.7
1	g	539	PRO	6.6
1	C	522	TRP	6.5
1	I	371	ALA	6.5
1	I	526	VAL	6.5
1	I	518	LEU	6.4
1	I	515	ALA	6.4
2	P	70	LEU	6.4
1	I	524	GLU	6.3
1	c	696	THR	6.2
1	g	515	ALA	6.2
2	N	81	TYR	6.2
1	Y	694	LYS	6.2
1	g	403	ILE	6.2
2	N	49	ALA	6.2
1	C	526	VAL	6.1
1	c	694	LYS	6.0
1	W	516	VAL	6.0
2	H	45	GLY	6.0
1	G	702	VAL	5.8
1	c	375	ASN	5.8
1	S	703	MET	5.8
2	Z	71	GLU	5.8
1	I	384	ILE	5.8
1	g	406	ASN	5.7
1	G	703	MET	5.6
1	g	517	ALA	5.5
1	W	405	GLU	5.5
1	I	385	TYR	5.5
1	C	518	LEU	5.5
1	I	383	LEU	5.4
1	c	783	ARG	5.4
1	Q	782	MET	5.4
1	Y	406	ASN	5.4
1	c	743	SER	5.3
2	R	152	GLU	5.3
1	c	703	MET	5.3
2	d	102	VAL	5.3
2	N	72	ARG	5.3
1	c	769	GLN	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	W	513	PRO	5.2
2	X	102	VAL	5.2
1	c	326	THR	5.2
1	c	327	LEU	5.2
2	N	73	TYR	5.2
1	C	519	LYS	5.2
1	G	692	ALA	5.2
1	g	610	GLN	5.2
1	c	306	ARG	5.2
1	g	594	MET	5.1
1	G	513	PRO	5.1
1	Q	703	MET	5.1
2	N	150	PHE	5.0
1	I	324	LEU	5.0
1	I	644	GLY	5.0
1	I	516	VAL	5.0
1	W	351	ARG	5.0
1	S	350	ALA	5.0
1	c	377	LYS	4.9
1	Q	219	TYR	4.9
1	I	373	VAL	4.8
1	c	744	GLN	4.8
1	I	519	LYS	4.8
2	h	169	LEU	4.8
1	I	514	SER	4.8
2	h	103	GLU	4.8
2	h	84	ALA	4.8
1	S	578	LEU	4.8
3	b	737	TYR	4.8
1	S	324	LEU	4.8
1	C	527	ARG	4.7
2	B	45	GLY	4.7
1	c	145	ILE	4.7
1	c	588	ILE	4.7
2	P	81	TYR	4.7
2	R	151	ILE	4.7
1	I	330	LYS	4.6
1	I	578	LEU	4.6
1	c	400	PRO	4.6
1	Q	578	LEU	4.6
2	Z	70	LEU	4.6
1	W	539	PRO	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	692	ALA	4.6
1	I	525	LYS	4.6
1	c	763	MET	4.6
2	X	77	THR	4.6
2	P	72	ARG	4.6
1	c	594	MET	4.6
2	X	73	TYR	4.6
1	C	367	PRO	4.5
2	N	74	ARG	4.5
1	c	773	LEU	4.5
1	C	516	VAL	4.5
1	I	527	ARG	4.5
2	R	120	MET	4.5
2	D	72	ARG	4.5
1	C	728	HIS	4.5
2	P	73	TYR	4.5
1	c	745	LEU	4.5
2	P	71	GLU	4.4
1	c	206	ILE	4.4
1	c	324	LEU	4.4
3	i	738	ILE	4.4
2	X	84	ALA	4.4
2	h	102	VAL	4.4
1	Y	693	PHE	4.4
2	X	103	GLU	4.4
2	T	46	VAL	4.4
2	T	74	ARG	4.4
1	g	350	ALA	4.4
1	g	744	GLN	4.4
2	h	83	GLY	4.4
2	J	69	GLY	4.4
1	c	707	ASP	4.3
1	S	351	ARG	4.3
1	c	722	LEU	4.3
1	C	382	TYR	4.3
1	I	599	VAL	4.3
1	W	404	PRO	4.3
1	C	366	VAL	4.3
1	g	742	GLY	4.3
2	N	121	LEU	4.3
1	Q	783	ARG	4.3
1	G	784	SER	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	d	103	GLU	4.3
2	P	103	GLU	4.3
1	S	321	GLY	4.3
2	D	69	GLY	4.3
2	h	46	VAL	4.3
1	C	385	TYR	4.3
2	h	165	PHE	4.3
1	c	718	MET	4.2
1	c	742	GLY	4.2
2	h	85	VAL	4.2
1	g	745	LEU	4.2
1	I	374	LEU	4.2
2	X	106	LEU	4.2
2	H	73	TYR	4.2
1	c	401	ALA	4.2
1	c	719	LEU	4.2
1	g	741	GLN	4.2
1	I	328	PRO	4.2
1	g	516	VAL	4.2
1	M	515	ALA	4.2
1	I	544	LEU	4.2
1	S	550	CYS	4.1
2	N	110	ARG	4.1
1	g	219	TYR	4.1
2	X	169	LEU	4.1
2	X	85	VAL	4.1
2	H	46	VAL	4.1
2	P	88	LEU	4.1
2	J	72	ARG	4.1
2	d	106	LEU	4.1
1	Q	324	LEU	4.1
3	i	746	MET	4.1
2	N	70	LEU	4.1
1	M	382	TYR	4.1
2	T	73	TYR	4.1
1	c	325	ALA	4.1
1	G	694	LYS	4.1
3	a	737	TYR	4.1
1	C	513	PRO	4.0
1	Q	577	PRO	4.0
2	h	13	LYS	4.0
1	O	550	CYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	g	364	VAL	4.0
1	I	329	THR	4.0
1	O	337	LEU	4.0
2	N	99	TYR	4.0
1	S	352	VAL	4.0
1	O	706	LEU	4.0
1	g	538	LEU	4.0
2	X	76	ILE	3.9
2	B	72	ARG	3.9
2	D	12	PHE	3.9
2	N	48	PHE	3.9
1	I	325	ALA	3.9
1	Y	324	LEU	3.9
1	C	524	GLU	3.9
1	S	218	ALA	3.9
2	P	49	ALA	3.9
1	I	648	VAL	3.9
1	g	159	TYR	3.9
1	g	586	LEU	3.9
1	Y	783	ARG	3.9
2	H	91	TYR	3.9
2	d	91	TYR	3.9
1	I	367	PRO	3.9
1	C	623	HIS	3.9
2	P	12	PHE	3.9
1	G	166	CYS	3.9
2	T	72	ARG	3.9
1	A	513	PRO	3.8
1	C	703	MET	3.8
1	Q	710	MET	3.8
1	O	623	HIS	3.8
2	d	72	ARG	3.8
1	M	513	PRO	3.8
2	R	103	GLU	3.8
3	b	734	LEU	3.8
1	S	320	ILE	3.8
2	h	12	PHE	3.8
1	Y	782	MET	3.8
1	C	374	LEU	3.8
2	N	103	GLU	3.8
1	c	350	ALA	3.8
1	W	216	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	70	LEU	3.8
2	H	131	LEU	3.8
2	N	77	THR	3.7
1	G	514	SER	3.7
1	g	513	PRO	3.7
2	d	173	TYR	3.7
1	W	514	SER	3.7
1	c	367	PRO	3.7
1	Y	405	GLU	3.7
2	P	102	VAL	3.7
1	I	539	PRO	3.7
2	N	88	LEU	3.7
1	G	515	ALA	3.7
1	W	535	TYR	3.7
1	M	744	GLN	3.7
1	Q	784	SER	3.7
2	H	72	ARG	3.7
1	I	672	HIS	3.7
1	M	324	LEU	3.7
1	C	373	VAL	3.7
1	c	764	SER	3.7
1	Y	784	SER	3.6
1	G	695	LEU	3.6
1	M	707	ASP	3.6
1	G	385	TYR	3.6
1	I	722	LEU	3.6
1	g	587	VAL	3.6
2	P	74	ARG	3.6
2	X	12	PHE	3.6
1	C	401	ALA	3.6
1	c	406	ASN	3.6
1	C	331	GLU	3.6
1	g	134	PHE	3.6
1	g	743	SER	3.6
1	Q	351	ARG	3.6
1	g	740	GLN	3.6
1	Q	623	HIS	3.6
1	c	130	LEU	3.6
2	N	62	ALA	3.6
1	I	219	TYR	3.6
2	R	123	GLY	3.6
2	T	45	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	341	LEU	3.6
1	C	675	PHE	3.6
3	f	737	TYR	3.6
1	C	330	LYS	3.5
2	R	106	LEU	3.5
1	S	702	VAL	3.5
1	I	543	LEU	3.5
2	P	17	ILE	3.5
1	C	219	TYR	3.5
1	O	594	MET	3.5
2	P	130	HIS	3.5
3	U	737	TYR	3.5
1	g	754	ILE	3.5
1	c	378	ASP	3.5
1	c	765	MET	3.5
1	G	600	ASN	3.5
1	c	148	LEU	3.5
1	g	382	TYR	3.5
1	W	406	ASN	3.5
2	P	89	LEU	3.5
1	A	370	GLN	3.5
1	G	374	LEU	3.5
1	c	749	HIS	3.5
1	Y	206	ILE	3.5
1	C	699	PHE	3.5
1	W	537	HIS	3.5
2	h	11	LEU	3.5
2	h	170	THR	3.5
2	N	119	ILE	3.5
2	Z	44	ILE	3.5
1	Y	306	ARG	3.4
2	B	119	ILE	3.4
2	N	87	ALA	3.4
3	a	740	ARG	3.4
1	g	673	ILE	3.4
1	g	548	VAL	3.4
2	D	80	TYR	3.4
1	A	164	LEU	3.4
1	W	538	LEU	3.4
1	M	706	LEU	3.4
3	i	742	ILE	3.4
1	I	545	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	81	TYR	3.4
2	d	116	ASN	3.4
1	A	703	MET	3.4
1	C	372	VAL	3.4
1	S	623	HIS	3.4
2	B	131	LEU	3.4
1	Q	695	LEU	3.4
1	c	784	SER	3.4
2	R	119	ILE	3.4
1	A	167	PHE	3.4
2	R	102	VAL	3.4
1	M	594	MET	3.3
1	g	585	ILE	3.3
1	I	699	PHE	3.3
2	N	151	ILE	3.3
1	O	219	TYR	3.3
2	N	12	PHE	3.3
2	R	38	LEU	3.3
2	H	150	PHE	3.3
1	C	544	LEU	3.3
1	W	134	PHE	3.3
1	A	784	SER	3.3
1	Q	702	VAL	3.3
2	d	141	ALA	3.3
3	i	741	ILE	3.3
1	c	353	TRP	3.3
1	I	331	GLU	3.3
2	D	62	ALA	3.3
1	G	544	LEU	3.3
3	a	734	LEU	3.3
1	O	707	ASP	3.3
1	I	381	PRO	3.3
2	h	80	TYR	3.3
1	O	702	VAL	3.3
1	c	354	LEU	3.3
1	I	645	TYR	3.3
2	P	50	THR	3.2
1	I	387	GLU	3.2
1	c	770	LEU	3.2
2	X	11	LEU	3.2
1	c	698	GLU	3.2
1	g	392	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	W	594	MET	3.2
2	Z	45	GLY	3.2
1	W	578	LEU	3.2
1	c	586	LEU	3.2
3	b	738	ILE	3.2
1	S	353	TRP	3.2
1	c	693	PHE	3.2
3	i	753	LEU	3.2
1	I	161	GLY	3.2
1	A	385	TYR	3.2
2	N	51	ARG	3.2
2	R	91	TYR	3.2
1	I	332	GLN	3.2
2	B	73	TYR	3.2
2	X	44	ILE	3.2
1	c	697	THR	3.2
2	X	53	ILE	3.2
2	h	53	ILE	3.2
1	c	131	LEU	3.2
2	B	91	TYR	3.2
1	C	629	GLU	3.2
1	G	404	PRO	3.2
1	M	318	MET	3.2
3	a	746	MET	3.2
1	c	615	LEU	3.2
2	P	62	ALA	3.2
1	W	741	GLN	3.2
1	g	402	ARG	3.1
1	I	321	GLY	3.1
1	O	703	MET	3.1
2	N	113	ALA	3.1
1	A	374	LEU	3.1
2	P	68	ALA	3.1
1	I	363	VAL	3.1
1	I	326	THR	3.1
1	Y	400	PRO	3.1
1	c	364	VAL	3.1
2	h	162	GLU	3.1
2	B	46	VAL	3.1
2	X	45	GLY	3.1
2	H	121	LEU	3.1
1	g	588	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	99	TYR	3.1
1	Q	704	GLY	3.1
1	S	216	LEU	3.1
1	Y	696	THR	3.1
1	C	212	CYS	3.1
1	Q	350	ALA	3.1
2	P	77	THR	3.1
2	h	106	LEU	3.1
1	c	746	PRO	3.1
1	I	600	ASN	3.1
1	g	535	TYR	3.1
1	W	740	GLN	3.1
1	W	742	GLY	3.1
1	c	352	VAL	3.1
2	X	165	PHE	3.1
1	M	623	HIS	3.1
2	h	73	TYR	3.1
3	b	744	ALA	3.1
1	I	521	PRO	3.1
1	S	373	VAL	3.1
2	X	6	ASP	3.1
1	g	578	LEU	3.1
1	Q	363	VAL	3.1
2	R	48	PHE	3.1
1	O	382	TYR	3.0
1	g	618	TYR	3.0
1	I	775	GLU	3.0
2	d	174	ARG	3.0
1	I	548	VAL	3.0
2	R	149	SER	3.0
2	D	131	LEU	3.0
2	H	44	ILE	3.0
1	S	577	PRO	3.0
2	H	94	ALA	3.0
1	O	372	VAL	3.0
1	W	348	LEU	3.0
3	i	752	ILE	3.0
1	c	349	PRO	3.0
2	X	72	ARG	3.0
1	M	516	VAL	3.0
1	C	515	ALA	3.0
1	I	642	CYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	g	534	PRO	3.0
1	O	651	LEU	3.0
1	I	571	TRP	3.0
1	Y	371	ALA	3.0
1	c	380	ALA	3.0
2	X	88	LEU	3.0
1	Y	722	LEU	3.0
1	G	159	TYR	3.0
1	C	344	LEU	3.0
2	T	77	THR	3.0
2	T	120	MET	3.0
1	Q	148	LEU	3.0
3	b	733	ARG	3.0
1	A	545	SER	3.0
1	M	371	ALA	3.0
1	C	384	ILE	3.0
1	I	643	ALA	3.0
1	W	517	ALA	3.0
2	H	90	VAL	3.0
2	R	94	ALA	3.0
2	T	39	GLU	3.0
1	g	370	GLN	3.0
2	N	102	VAL	3.0
1	c	363	VAL	3.0
2	R	46	VAL	3.0
1	O	517	ALA	3.0
2	R	93	ILE	3.0
1	S	635	GLN	2.9
2	N	46	VAL	2.9
3	b	735	GLN	2.9
1	I	546	VAL	2.9
1	I	344	LEU	2.9
1	I	598	VAL	2.9
2	P	46	VAL	2.9
1	c	619	PHE	2.9
1	M	334	THR	2.9
2	P	87	ALA	2.9
1	W	159	TYR	2.9
1	M	337	LEU	2.9
2	R	121	LEU	2.9
1	G	167	PHE	2.9
2	P	96	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	c	774	VAL	2.9
1	S	615	LEU	2.9
1	I	703	MET	2.9
2	X	51	ARG	2.9
1	W	363	VAL	2.9
1	S	371	ALA	2.9
1	c	141	ILE	2.9
2	P	119	ILE	2.9
2	h	45	GLY	2.9
1	S	782	MET	2.9
1	C	706	LEU	2.9
1	Q	585	ILE	2.9
1	C	543	LEU	2.9
1	O	318	MET	2.9
1	O	373	VAL	2.9
1	S	710	MET	2.9
2	d	170	THR	2.9
1	W	349	PRO	2.9
1	W	754	ILE	2.9
1	c	138	LEU	2.9
2	N	38	LEU	2.9
2	P	131	LEU	2.9
1	A	702	VAL	2.9
1	I	629	GLU	2.9
1	Q	651	LEU	2.9
1	Y	141	ILE	2.9
2	X	83	GLY	2.9
1	M	219	TYR	2.9
1	S	555	ARG	2.8
1	S	722	LEU	2.8
1	g	180	LEU	2.8
1	S	627	THR	2.8
2	H	80	TYR	2.8
2	J	81	TYR	2.8
2	J	70	LEU	2.8
3	L	746	MET	2.8
1	C	329	THR	2.8
2	P	63	GLN	2.8
1	O	134	PHE	2.8
1	A	373	VAL	2.8
1	A	691	SER	2.8
1	c	766	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	71	GLU	2.8
1	M	317	LEU	2.8
1	Y	744	GLN	2.8
2	B	92	ASP	2.8
2	P	106	LEU	2.8
1	I	366	VAL	2.8
1	I	623	HIS	2.8
1	S	372	VAL	2.8
1	c	370	GLN	2.8
2	H	134	VAL	2.8
1	c	241	LEU	2.8
2	d	110	ARG	2.8
3	i	740	ARG	2.8
1	Q	353	TRP	2.8
1	W	576	VAL	2.8
1	S	675	PHE	2.8
2	P	48	PHE	2.8
1	W	147	TYR	2.8
1	S	576	VAL	2.8
1	g	139	PHE	2.8
3	a	753	LEU	2.8
1	C	695	LEU	2.8
1	G	370	GLN	2.8
3	E	717	ARG	2.8
1	c	626	TYR	2.8
2	J	12	PHE	2.8
1	C	727	LYS	2.8
1	M	517	ALA	2.8
1	S	672	HIS	2.8
1	C	598	VAL	2.8
1	C	370	GLN	2.8
1	g	615	LEU	2.8
2	H	178	GLN	2.8
1	S	340	GLU	2.8
1	Q	182	MET	2.8
1	O	744	GLN	2.8
1	Q	640	GLN	2.8
2	R	150	PHE	2.8
1	S	374	LEU	2.8
2	d	71	GLU	2.8
1	G	355	PRO	2.8
2	R	96	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	63	GLN	2.8
3	b	736	ASP	2.8
2	X	62	ALA	2.8
1	c	723	ILE	2.8
1	g	129	TRP	2.8
2	D	63	GLN	2.7
1	C	387	GLU	2.7
1	S	323	ARG	2.7
3	K	722	GLU	2.7
2	d	145	LYS	2.7
1	Q	650	TYR	2.7
1	g	363	VAL	2.7
2	d	137	ASP	2.7
3	b	741	ILE	2.7
1	C	525	LYS	2.7
1	W	347	LYS	2.7
2	R	110	ARG	2.7
1	c	180	LEU	2.7
1	A	694	LYS	2.7
2	Z	80	TYR	2.7
1	Y	241	LEU	2.7
2	N	109	LEU	2.7
2	P	16	LEU	2.7
1	C	349	PRO	2.7
1	C	535	TYR	2.7
1	A	578	LEU	2.7
2	B	70	LEU	2.7
2	H	133	ALA	2.7
3	i	734	LEU	2.7
1	S	194	ILE	2.7
2	T	123	GLY	2.7
1	S	784	SER	2.7
2	N	120	MET	2.7
3	i	744	ALA	2.7
2	D	50	THR	2.7
1	I	158	ALA	2.7
1	Q	762	HIS	2.7
2	T	88	LEU	2.7
2	P	120	MET	2.7
2	Z	46	VAL	2.7
1	W	660	GLY	2.7
2	B	81	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	739	MET	2.7
1	C	548	VAL	2.7
1	I	737	GLU	2.7
1	S	363	VAL	2.7
1	W	364	VAL	2.7
1	Y	373	VAL	2.7
1	G	164	LEU	2.7
1	c	385	TYR	2.7
2	X	80	TYR	2.7
1	I	386	VAL	2.7
1	C	630	ALA	2.7
1	W	180	LEU	2.7
1	g	400	PRO	2.7
2	P	94	ALA	2.7
1	C	622	GLU	2.7
1	S	704	GLY	2.7
2	P	67	THR	2.7
1	Y	130	LEU	2.7
1	S	148	LEU	2.7
2	N	89	LEU	2.7
1	c	129	TRP	2.7
2	h	63	GLN	2.7
1	M	615	LEU	2.7
1	I	647	LEU	2.6
1	S	695	LEU	2.6
2	P	150	PHE	2.6
2	R	45	GLY	2.6
2	R	153	THR	2.6
1	O	406	ASN	2.6
1	c	711	PHE	2.6
2	N	149	SER	2.6
1	g	747	CYS	2.6
2	J	27	LEU	2.6
1	A	219	TYR	2.6
1	C	666	ALA	2.6
1	G	783	ARG	2.6
1	Q	777	MET	2.6
1	Y	706	LEU	2.6
3	e	746	MET	2.6
1	Q	131	LEU	2.6
1	S	382	TYR	2.6
1	O	513	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	c	638	PHE	2.6
1	S	714	TYR	2.6
2	P	129	ARG	2.6
2	d	73	TYR	2.6
1	W	587	VAL	2.6
1	Y	703	MET	2.6
1	I	520	GLU	2.6
1	c	362	HIS	2.6
1	Q	576	VAL	2.6
1	g	576	VAL	2.6
2	h	76	ILE	2.6
1	g	554	LEU	2.6
2	T	41	LYS	2.6
1	C	642	CYS	2.6
2	d	115	SER	2.6
2	h	16	LEU	2.6
2	J	150	PHE	2.6
2	P	32	THR	2.6
1	A	514	SER	2.6
1	Q	630	ALA	2.6
2	H	89	LEU	2.6
1	M	320	ILE	2.6
1	W	743	SER	2.6
1	O	161	GLY	2.6
1	I	375	ASN	2.6
1	C	725	ALA	2.6
1	G	522	TRP	2.6
1	Q	747	CYS	2.6
1	Y	354	LEU	2.6
2	X	46	VAL	2.6
2	X	52	SER	2.6
1	M	338	ILE	2.6
1	g	660	GLY	2.6
2	d	62	ALA	2.6
1	O	663	LEU	2.6
1	Q	138	LEU	2.6
1	Q	385	TYR	2.6
1	Q	619	PHE	2.6
1	I	630	ALA	2.6
1	W	574	GLU	2.6
2	P	45	GLY	2.6
1	Q	717	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	91	TYR	2.6
2	R	124	ASN	2.6
2	R	90	VAL	2.5
1	C	729	MET	2.5
1	c	725	ALA	2.5
1	C	571	TRP	2.5
1	W	581	LYS	2.5
1	I	376	SER	2.5
1	I	401	ALA	2.5
1	M	702	VAL	2.5
1	O	164	LEU	2.5
1	O	578	LEU	2.5
1	c	373	VAL	2.5
2	B	150	PHE	2.5
2	T	70	LEU	2.5
2	h	100	GLU	2.5
2	T	178	GLN	2.5
2	d	99	TYR	2.5
2	R	89	LEU	2.5
2	P	117	ILE	2.5
1	A	599	VAL	2.5
2	X	87	ALA	2.5
1	G	395	ASP	2.5
1	C	644	GLY	2.5
1	G	704	GLY	2.5
1	O	551	GLY	2.5
1	Q	594	MET	2.5
1	g	739	MET	2.5
2	R	80	TYR	2.5
1	c	134	PHE	2.5
1	Q	352	VAL	2.5
2	Z	74	ARG	2.5
1	Q	599	VAL	2.5
3	U	742	ILE	2.5
3	b	745	ILE	2.5
1	O	371	ALA	2.5
1	c	351	ARG	2.5
2	B	69	GLY	2.5
1	O	664	LEU	2.5
2	P	109	LEU	2.5
2	h	77	THR	2.5
1	I	529	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	185	HIS	2.5
1	W	403	ILE	2.5
1	g	351	ARG	2.5
3	j	737	TYR	2.5
1	I	327	LEU	2.5
1	A	623	HIS	2.5
1	I	649	CYS	2.5
2	B	120	MET	2.5
2	X	61	LYS	2.5
1	A	159	TYR	2.5
2	T	38	LEU	2.5
2	D	39	GLU	2.5
1	c	214	LEU	2.5
2	R	99	TYR	2.5
1	c	699	PHE	2.5
3	U	756	LYS	2.5
1	g	557	GLU	2.5
2	N	122	VAL	2.5
2	R	50	THR	2.5
2	Z	77	THR	2.5
1	Q	601	ALA	2.5
1	S	220	SER	2.5
2	d	178	GLN	2.5
1	Y	375	ASN	2.5
2	d	45	GLY	2.5
1	I	749	HIS	2.5
1	g	138	LEU	2.5
2	T	50	THR	2.5
1	C	529	ILE	2.5
2	P	144	GLU	2.4
1	c	328	PRO	2.4
3	V	733	ARG	2.4
3	b	740	ARG	2.4
1	I	651	LEU	2.4
1	O	344	LEU	2.4
1	Q	374	LEU	2.4
1	Y	404	PRO	2.4
2	T	40	SER	2.4
2	N	15	VAL	2.4
1	Q	571	TRP	2.4
1	c	176	LEU	2.4
1	g	380	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	d	138	GLU	2.4
1	C	754	ILE	2.4
3	a	741	ILE	2.4
1	S	215	LEU	2.4
1	S	619	PHE	2.4
2	h	67	THR	2.4
1	Q	587	VAL	2.4
1	Y	515	ALA	2.4
1	W	139	PHE	2.4
1	A	714	TYR	2.4
1	C	148	LEU	2.4
1	Q	639	VAL	2.4
1	S	587	VAL	2.4
2	h	14	VAL	2.4
1	C	381	PRO	2.4
2	D	73	TYR	2.4
1	S	699	PHE	2.4
1	G	599	VAL	2.4
1	I	577	PRO	2.4
2	h	88	LEU	2.4
3	a	733	ARG	2.4
1	I	380	ALA	2.4
1	c	213	ALA	2.4
1	S	513	PRO	2.4
3	E	718	ASP	2.4
1	O	518	LEU	2.4
1	Q	164	LEU	2.4
1	g	661	ASN	2.4
1	S	571	TRP	2.4
1	g	184	ILE	2.4
1	C	383	LEU	2.4
1	I	323	ARG	2.4
1	W	355	PRO	2.4
1	Y	351	ARG	2.4
3	a	735	GLN	2.4
3	U	741	ILE	2.4
1	C	652	LEU	2.4
1	S	706	LEU	2.4
1	M	550	CYS	2.4
2	N	96	HIS	2.4
1	Y	327	LEU	2.4
1	g	131	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	122	VAL	2.4
1	G	601	ALA	2.4
1	M	385	TYR	2.4
2	R	81	TYR	2.4
2	d	136	THR	2.4
3	F	746	MET	2.4
2	D	11	LEU	2.4
2	X	63	GLN	2.4
1	C	784	SER	2.4
1	S	599	VAL	2.4
1	O	130	LEU	2.4
1	g	748	PHE	2.4
2	P	148	LEU	2.4
1	O	330	LYS	2.4
1	M	586	LEU	2.4
1	O	324	LEU	2.4
1	C	371	ALA	2.4
1	G	701	ASP	2.4
2	N	140	ARG	2.4
2	R	72	ARG	2.4
1	Q	638	PHE	2.4
1	g	514	SER	2.3
1	W	544	LEU	2.3
1	Y	401	ALA	2.3
2	N	17	ILE	2.3
2	P	118	VAL	2.3
1	M	548	VAL	2.3
2	P	11	LEU	2.3
1	W	534	PRO	2.3
2	T	96	HIS	2.3
1	Y	326	THR	2.3
2	P	85	VAL	2.3
2	R	178	GLN	2.3
2	X	70	LEU	2.3
1	S	385	TYR	2.3
1	Y	219	TYR	2.3
2	H	132	ARG	2.3
2	J	57	GLY	2.3
1	Q	194	ILE	2.3
1	C	364	VAL	2.3
1	C	514	SER	2.3
1	O	341	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	765	MET	2.3
1	Y	588	ILE	2.3
1	I	528	ARG	2.3
1	Q	306	ARG	2.3
2	N	45	GLY	2.3
1	C	615	LEU	2.3
1	M	344	LEU	2.3
1	Q	732	VAL	2.3
1	W	387	GLU	2.3
1	Q	735	ILE	2.3
1	S	364	VAL	2.3
1	C	599	VAL	2.3
2	T	102	VAL	2.3
2	h	81	TYR	2.3
2	T	44	ILE	2.3
1	O	334	THR	2.3
1	c	323	ARG	2.3
1	W	392	GLU	2.3
2	P	91	TYR	2.3
3	i	745	ILE	2.3
1	Q	668	GLY	2.3
1	W	131	LEU	2.3
1	C	356	THR	2.3
1	Q	311	ARG	2.3
1	C	567	LEU	2.3
1	Q	321	GLY	2.3
1	c	721	GLY	2.3
2	N	86	GLY	2.3
2	d	144	GLU	2.3
2	d	171	GLU	2.3
3	U	734	LEU	2.3
1	g	369	THR	2.3
1	I	180	LEU	2.3
1	M	618	TYR	2.3
1	W	615	LEU	2.3
1	c	571	TRP	2.3
1	S	783	ARG	2.3
1	g	581	LYS	2.3
1	c	210	LEU	2.3
1	M	703	MET	2.3
1	I	369	THR	2.3
1	C	549	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	322	LYS	2.3
2	h	61	LYS	2.3
1	S	337	LEU	2.3
1	W	130	LEU	2.3
1	g	577	PRO	2.3
2	B	90	VAL	2.3
2	D	51	ARG	2.3
2	d	140	ARG	2.3
1	A	515	ALA	2.3
1	O	317	LEU	2.3
2	T	106	LEU	2.3
1	C	594	MET	2.2
1	Q	556	GLN	2.2
1	I	212	CYS	2.2
1	c	317	LEU	2.2
1	c	550	CYS	2.2
1	c	772	LEU	2.2
1	g	348	LEU	2.2
2	T	152	GLU	2.2
1	g	699	PHE	2.2
2	X	74	ARG	2.2
1	M	745	LEU	2.2
2	N	106	LEU	2.2
1	M	675	PHE	2.2
1	S	535	TYR	2.2
1	Y	699	PHE	2.2
1	c	149	TYR	2.2
1	S	732	VAL	2.2
1	A	737	GLU	2.2
1	g	675	PHE	2.2
1	A	544	LEU	2.2
1	O	615	LEU	2.2
1	S	193	ALA	2.2
2	B	88	LEU	2.2
1	A	701	ASP	2.2
2	R	165	PHE	2.2
1	M	718	MET	2.2
1	M	728	HIS	2.2
2	D	27	LEU	2.2
1	M	138	LEU	2.2
1	S	322	LYS	2.2
1	A	731	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	b	722	GLU	2.2
1	G	369	THR	2.2
1	W	540	ASN	2.2
2	D	83	GLY	2.2
1	Q	384	ILE	2.2
1	C	542	ARG	2.2
1	C	749	HIS	2.2
1	S	379	LYS	2.2
1	W	138	LEU	2.2
1	W	586	LEU	2.2
2	h	38	LEU	2.2
2	D	150	PHE	2.2
1	c	768	GLU	2.2
1	W	212	CYS	2.2
1	C	672	HIS	2.2
1	g	352	VAL	2.2
3	U	730	ILE	2.2
1	A	197	TYR	2.2
2	H	87	ALA	2.2
1	M	330	LYS	2.2
1	M	729	MET	2.2
1	Q	694	LYS	2.2
1	g	694	LYS	2.2
2	B	67	THR	2.2
2	R	98	THR	2.2
1	C	648	VAL	2.2
1	W	219	TYR	2.2
2	P	75	ALA	2.2
2	P	83	GLY	2.2
2	P	121	LEU	2.2
2	N	64	ILE	2.2
1	I	400	PRO	2.2
2	H	81	TYR	2.2
1	Y	745	LEU	2.2
1	g	773	LEU	2.2
2	D	76	ILE	2.2
2	h	44	ILE	2.2
1	C	743	SER	2.2
1	M	346	HIS	2.2
1	c	618	TYR	2.2
2	R	155	ALA	2.2
1	Q	567	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	122	VAL	2.2
3	b	730	ILE	2.2
1	g	130	LEU	2.2
1	C	744	GLN	2.2
1	G	699	PHE	2.2
1	S	604	ILE	2.2
1	S	761	PHE	2.2
1	c	183	TYR	2.2
2	h	15	VAL	2.2
1	S	586	LEU	2.2
1	c	403	ILE	2.2
2	T	27	LEU	2.2
1	I	542	ARG	2.2
1	G	782	MET	2.1
2	T	89	LEU	2.1
1	I	232	ARG	2.1
1	G	545	SER	2.1
1	S	735	ILE	2.1
1	Q	699	PHE	2.1
1	M	743	SER	2.1
1	Q	307	LEU	2.1
2	H	92	ASP	2.1
1	G	306	ARG	2.1
1	W	777	MET	2.1
1	A	202	CYS	2.1
1	S	212	CYS	2.1
2	H	151	ILE	2.1
2	X	13	LYS	2.1
2	X	28	LEU	2.1
1	I	364	VAL	2.1
1	c	139	PHE	2.1
1	W	703	MET	2.1
1	C	213	ALA	2.1
1	C	580	ILE	2.1
1	g	555	ARG	2.1
1	C	711	PHE	2.1
1	Q	722	LEU	2.1
2	P	38	LEU	2.1
1	g	537	HIS	2.1
3	i	737	TYR	2.1
1	A	326	THR	2.1
1	C	578	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	W	362	HIS	2.1
1	C	596	GLU	2.1
1	O	379	LYS	2.1
1	g	549	LYS	2.1
1	Q	760	ARG	2.1
2	B	68	ALA	2.1
2	N	14	VAL	2.1
1	I	567	LEU	2.1
2	R	148	LEU	2.1
1	Q	744	GLN	2.1
1	M	699	PHE	2.1
1	c	382	TYR	2.1
1	c	627	THR	2.1
1	g	362	HIS	2.1
2	H	88	LEU	2.1
1	I	622	GLU	2.1
1	A	529	ILE	2.1
1	M	215	LEU	2.1
1	S	559	LEU	2.1
1	W	588	ILE	2.1
1	c	714	TYR	2.1
2	d	70	LEU	2.1
1	W	185	HIS	2.1
1	S	567	LEU	2.1
2	J	131	LEU	2.1
1	C	748	PHE	2.1
1	c	682	SER	2.1
2	B	93	ILE	2.1
1	c	781	SER	2.1
1	Q	615	LEU	2.1
1	Q	745	LEU	2.1
1	W	356	THR	2.1
2	X	38	LEU	2.1
1	I	195	LYS	2.1
1	M	587	VAL	2.1
2	P	86	GLY	2.1
2	d	107	LYS	2.1
2	D	94	ALA	2.1
1	A	704	GLY	2.1
1	g	558	LEU	2.1
2	R	131	LEU	2.1
1	Y	702	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	237	ARG	2.1
1	c	179	LEU	2.1
3	K	718	ASP	2.1
1	M	514	SER	2.1
2	h	33	ARG	2.1
1	C	707	ASP	2.1
1	W	386	VAL	2.1
2	D	84	ALA	2.1
1	I	159	TYR	2.1
1	W	699	PHE	2.1
1	Y	615	LEU	2.1
2	D	152	GLU	2.1
1	Y	594	MET	2.0
1	c	777	MET	2.0
1	O	699	PHE	2.0
1	c	184	ILE	2.0
2	Z	53	ILE	2.0
1	g	367	PRO	2.0
1	g	746	PRO	2.0
1	Y	672	HIS	2.0
2	J	39	GLU	2.0
1	Y	359	PHE	2.0
2	T	68	ALA	2.0
2	h	150	PHE	2.0
2	Z	81	TYR	2.0
1	c	368	HIS	2.0
2	X	86	GLY	2.0
3	a	738	ILE	2.0
3	j	741	ILE	2.0
1	Q	652	LEU	2.0
2	X	33	ARG	2.0
2	Z	99	TYR	2.0
2	h	82	ARG	2.0
1	C	531	GLU	2.0
1	I	754	ILE	2.0
1	C	375	ASN	2.0
1	A	237	ARG	2.0
1	S	601	ALA	2.0
2	D	151	ILE	2.0
2	J	13	LYS	2.0
1	A	594	MET	2.0
1	W	736	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	g	148	LEU	2.0
2	R	27	LEU	2.0
1	Y	642	CYS	2.0
1	Q	570	ILE	2.0
2	B	151	ILE	2.0
2	N	44	ILE	2.0
3	U	738	ILE	2.0
1	M	373	VAL	2.0
1	Q	189	ASP	2.0
2	J	19	ASP	2.0
1	G	710	MET	2.0
1	O	374	LEU	2.0
1	Q	664	LEU	2.0
1	S	544	LEU	2.0
1	g	128	SER	2.0
1	I	193	ALA	2.0
2	R	100	GLU	2.0
2	h	62	ALA	2.0
1	Q	216	LEU	2.0
1	S	349	PRO	2.0
1	S	383	LEU	2.0
1	W	546	VAL	2.0
1	O	564	LEU	2.0
1	W	773	LEU	2.0
2	R	109	LEU	2.0
1	A	695	LEU	2.0
1	O	675	PHE	2.0
1	Q	672	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MG	d	2001	1/1	0.25	1.96	167,167,167,167	0
6	MG	D	2001	1/1	0.21	-0.33	64,64,64,64	0
5	GSP	Z	2000	32/32	0.22	-0.41	176,212,274,298	0
5	GSP	P	2000	32/32	0.24	-0.43	111,168,247,275	0
5	GSP	X	2000	32/32	0.24	-0.53	134,226,322,330	0
5	GSP	d	2000	32/32	0.17	-0.54	174,212,349,391	0
5	GSP	H	2000	32/32	0.25	-0.56	141,183,247,282	0
5	GSP	N	2000	32/32	0.23	-0.61	97,151,255,301	0
5	GSP	h	2000	32/32	0.22	-0.66	123,249,350,363	0
5	GSP	J	2000	32/32	0.26	-0.67	94,165,285,323	0
5	GSP	T	2000	32/32	0.26	-0.72	123,205,238,264	0
5	GSP	B	2000	32/32	0.22	-0.73	141,197,232,249	0
6	MG	B	2001	1/1	0.21	-0.78	159,159,159,159	0
5	GSP	D	2000	32/32	0.25	-0.81	110,193,250,272	0
6	MG	J	2001	1/1	0.16	-1.00	142,142,142,142	0
5	GSP	R	2000	32/32	0.21	-1.03	108,197,262,274	0
6	MG	T	2001	1/1	0.14	-1.17	127,127,127,127	0
6	MG	R	2001	1/1	0.13	-1.17	106,106,106,106	0
6	MG	H	2001	1/1	0.14	-1.19	139,139,139,139	0
6	MG	N	2001	1/1	0.11	-1.20	240,240,240,240	0
6	MG	P	2001	1/1	0.12	-1.21	244,244,244,244	0
6	MG	Z	2001	1/1	0.13	-1.43	178,178,178,178	0
6	MG	h	2001	1/1	0.09	-1.85	190,190,190,190	0
6	MG	X	2001	1/1	0.10	-2.01	255,255,255,255	0
4	093	I	2002	24/24	-	-	60,76,105,130	24
4	093	S	2002	24/24	-	-	60,76,105,130	24
4	093	Q	2002	24/24	-	-	60,76,105,130	24
4	093	W	2002	24/24	-	-	60,76,105,130	24
4	093	G	2002	24/24	-	-	60,76,105,130	24
4	093	Y	2002	24/24	-	-	60,76,105,130	24
4	093	g	2002	24/24	-	-	60,76,105,130	24
4	093	O	2002	24/24	-	-	60,76,105,130	24
4	093	A	2002	24/24	-	-	60,76,105,130	24
4	093	c	2002	24/24	-	-	60,76,105,130	24
4	093	M	2002	24/24	-	-	60,76,105,130	24
4	093	C	2002	24/24	-	-	60,76,105,130	24

6.5 Other polymers ⓘ

There are no such residues in this entry.