



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:13 PM UTC

PDB ID : 3NG9 / pdb_00003ng9
Title : Structure to Function Correlations for Adeno-associated Virus Serotype 1
Authors : Govindasamy, L.; Miller, E.B.; Gurda, B.; McKenna, R.; Zolotukhin, S.; Muzy-
czka, N.; Agbandje-McKenna, M.
Deposited on : 2010-06-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

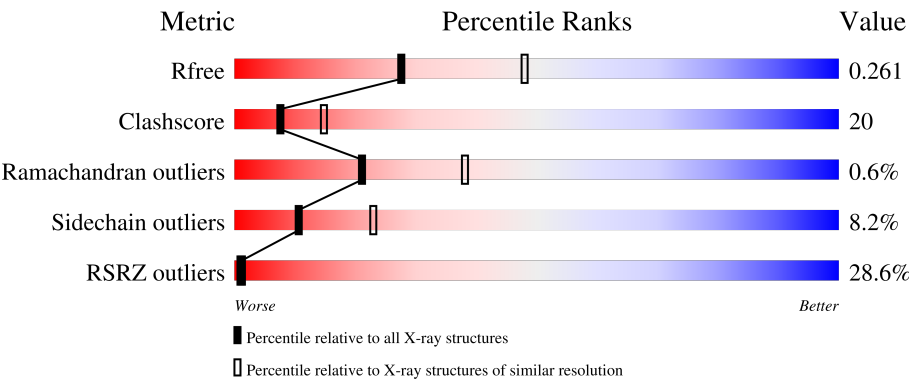
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	7% 46%20%29%
1	B	736	15% 46%20%29%
1	C	736	20% 47%20%29%
1	D	736	12% 45%21%29%
1	E	736	30% 46%21%29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	736	16% 45% 22% • 29%
1	G	736	24% 45% 22% • 29%
1	H	736	12% 46% 20% • • 29%
1	I	736	24% 45% 21% • 29%
1	J	736	42% 49% 18% • 29%

2 Entry composition

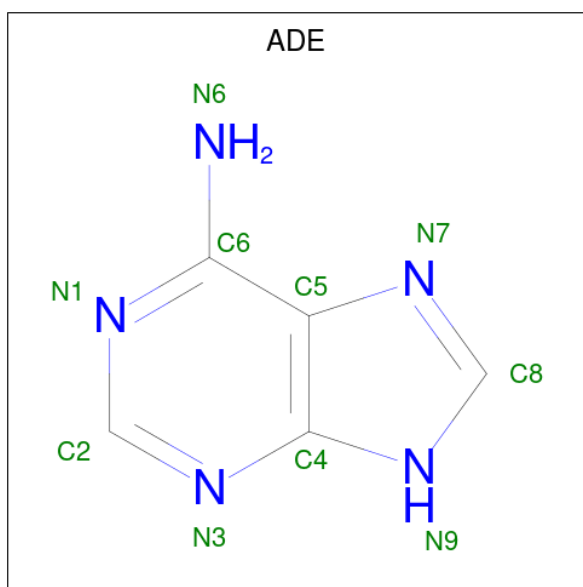
There are 4 unique types of molecules in this entry. The entry contains 42680 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein.

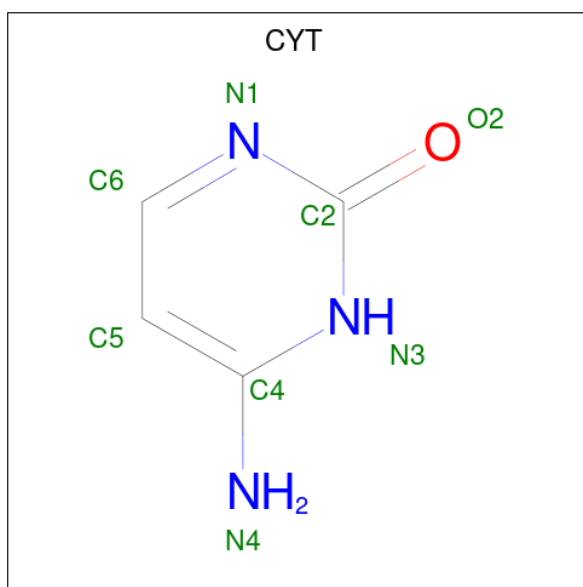
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	B	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	C	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	D	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	E	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	F	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	G	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	H	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	I	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	J	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			

- Molecule 2 is ADENINE (CCD ID: ADE) (formula: C₅H₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	5	5		
2	B	1	Total	C	N	0	0
			10	5	5		
2	C	1	Total	C	N	0	0
			10	5	5		
2	D	1	Total	C	N	0	0
			10	5	5		
2	E	1	Total	C	N	0	0
			10	5	5		
2	F	1	Total	C	N	0	0
			10	5	5		
2	G	1	Total	C	N	0	0
			10	5	5		
2	H	1	Total	C	N	0	0
			10	5	5		
2	I	1	Total	C	N	0	0
			10	5	5		
2	J	1	Total	C	N	0	0
			10	5	5		

- Molecule 3 is 6-AMINOPYRIMIDIN-2(1H)-ONE (CCD ID: CYT) (formula: $C_4H_5N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	3	1		
3	B	1	Total	C	N	O	0	0
			8	4	3	1		
3	B	1	Total	C	N	O	0	0
			8	4	3	1		
3	C	1	Total	C	N	O	0	0
			8	4	3	1		
3	D	1	Total	C	N	O	0	0
			8	4	3	1		
3	E	1	Total	C	N	O	0	0
			8	4	3	1		
3	F	1	Total	C	N	O	0	0
			8	4	3	1		
3	H	1	Total	C	N	O	0	0
			8	4	3	1		
3	I	1	Total	C	N	O	0	0
			8	4	3	1		
3	J	1	Total	C	N	O	0	0
			8	4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		
4	B	130	Total	O	0	0
			130	130		

Continued on next page...

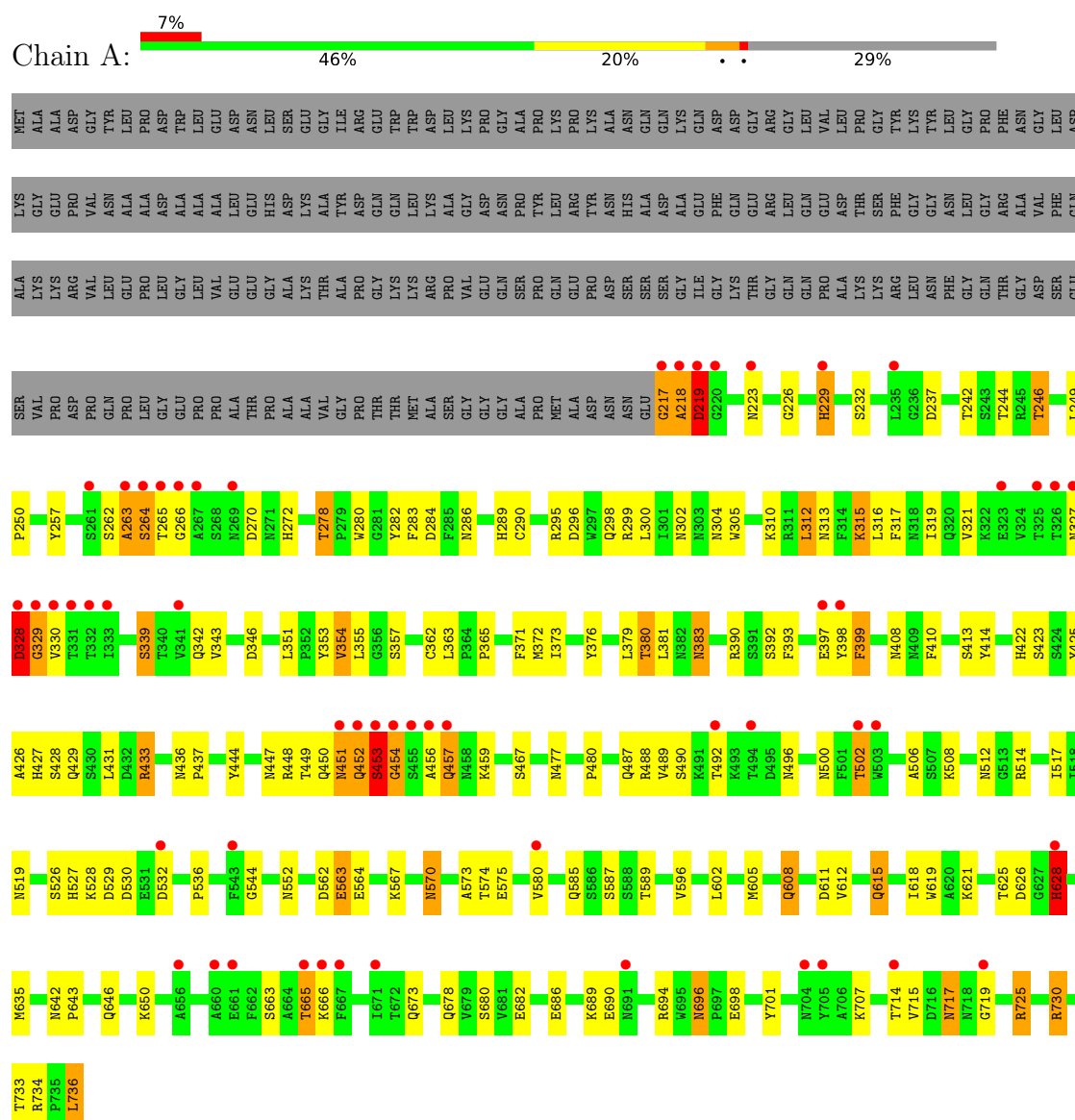
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	128	Total 128	O 128	0	0
4	D	131	Total 131	O 131	0	0
4	E	133	Total 133	O 133	0	0
4	F	131	Total 131	O 131	0	0
4	G	127	Total 127	O 127	0	0
4	H	130	Total 130	O 130	0	0
4	I	130	Total 130	O 130	0	0
4	J	129	Total 129	O 129	0	0

3 Residue-property plots

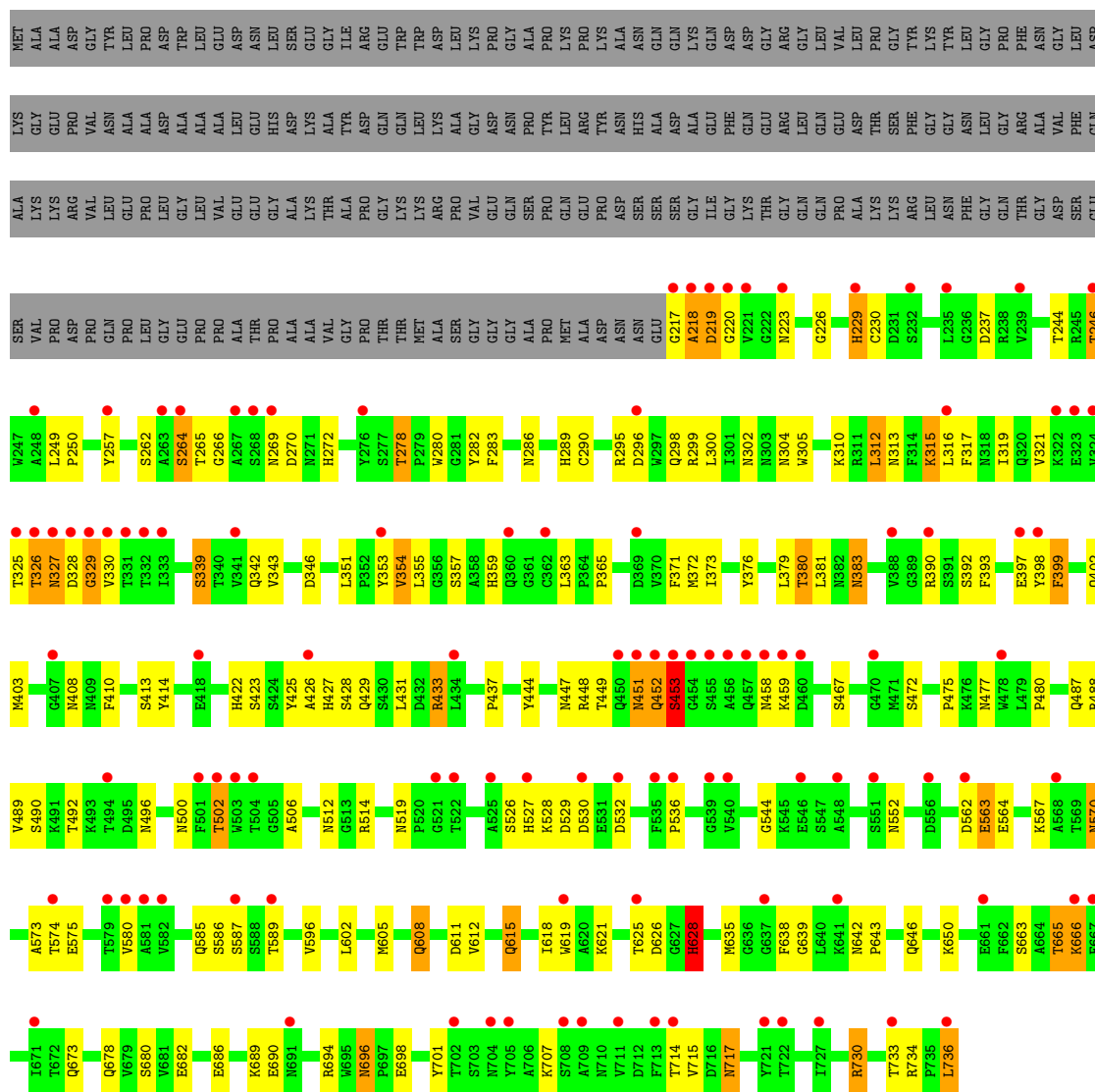
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Capsid protein

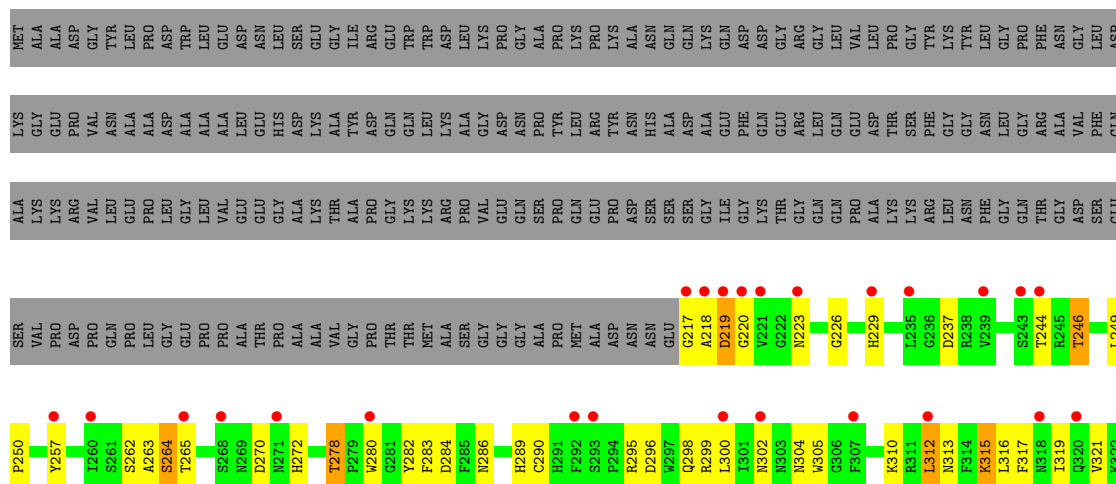


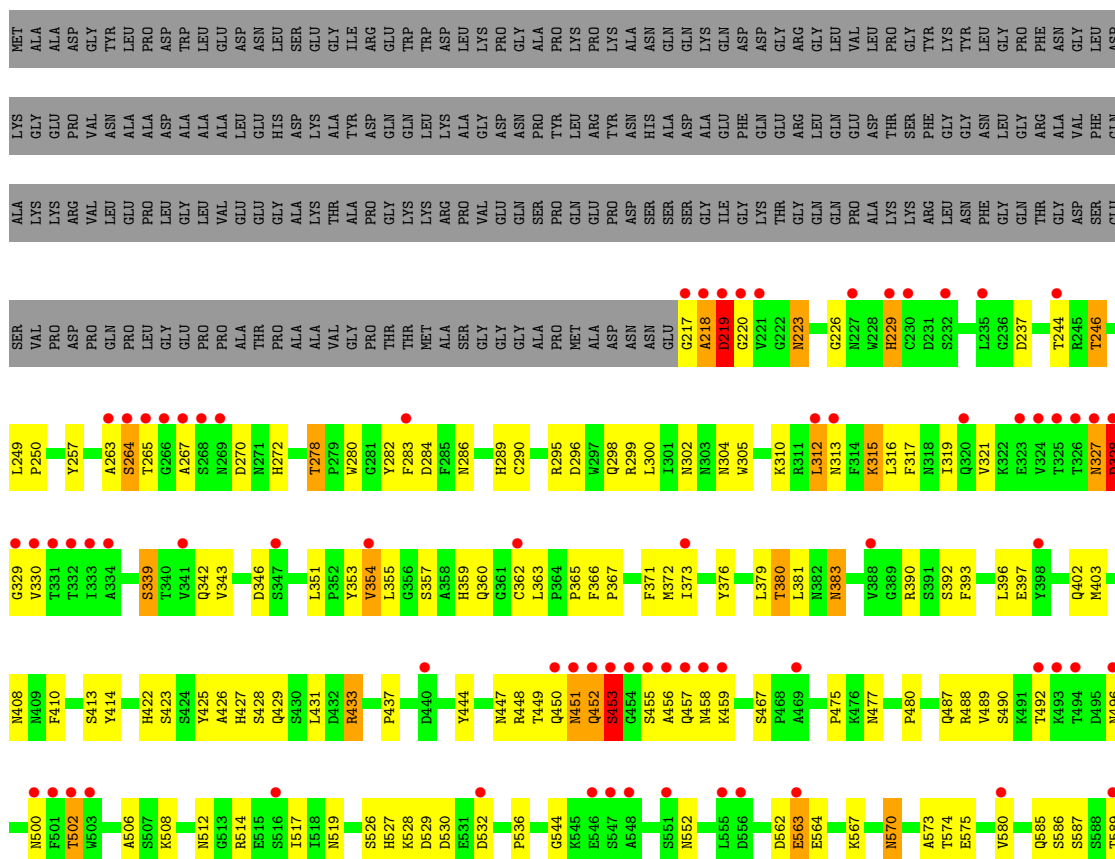
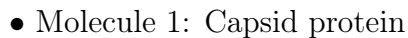
• Molecule 1: Capsid protein

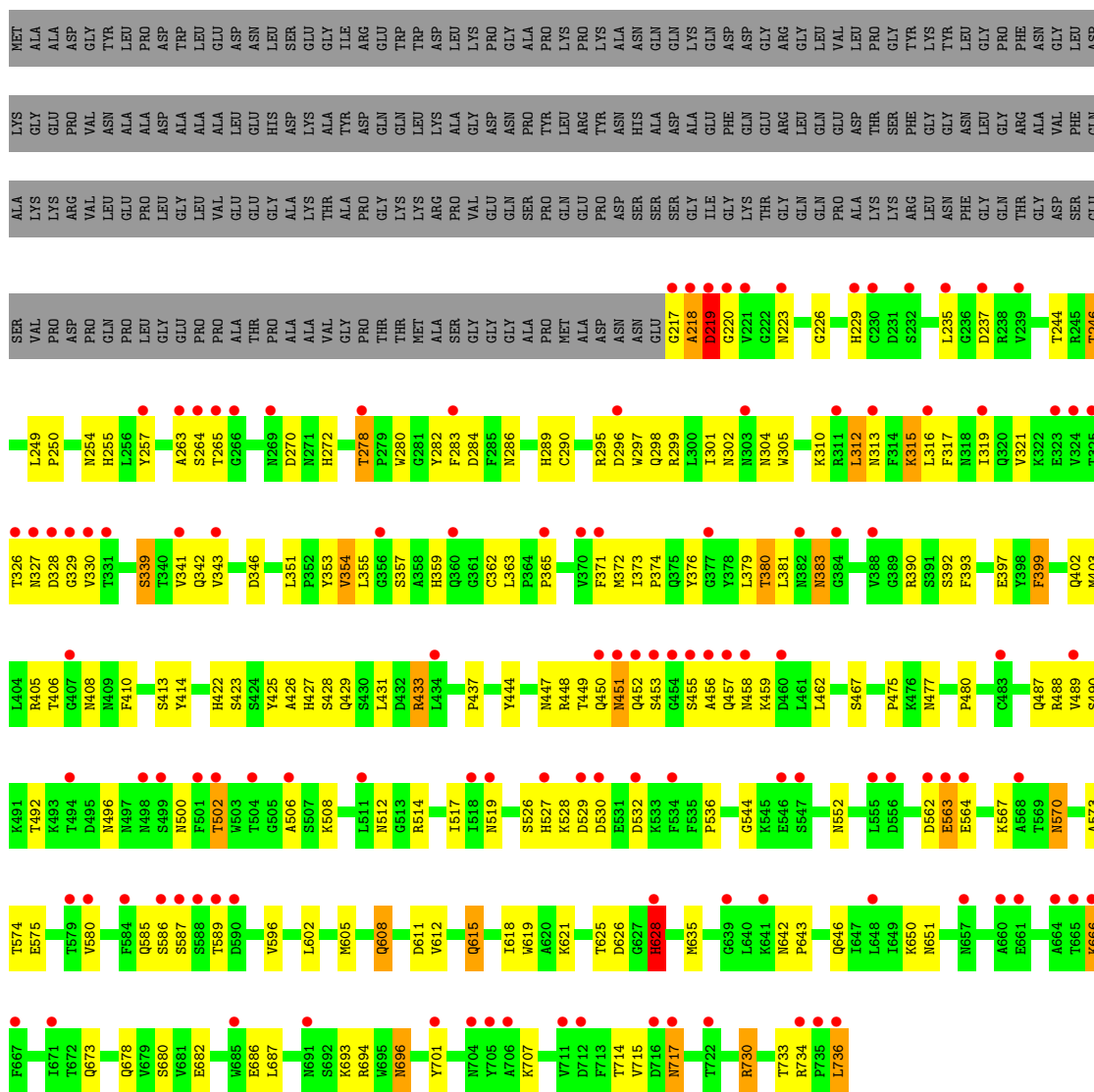




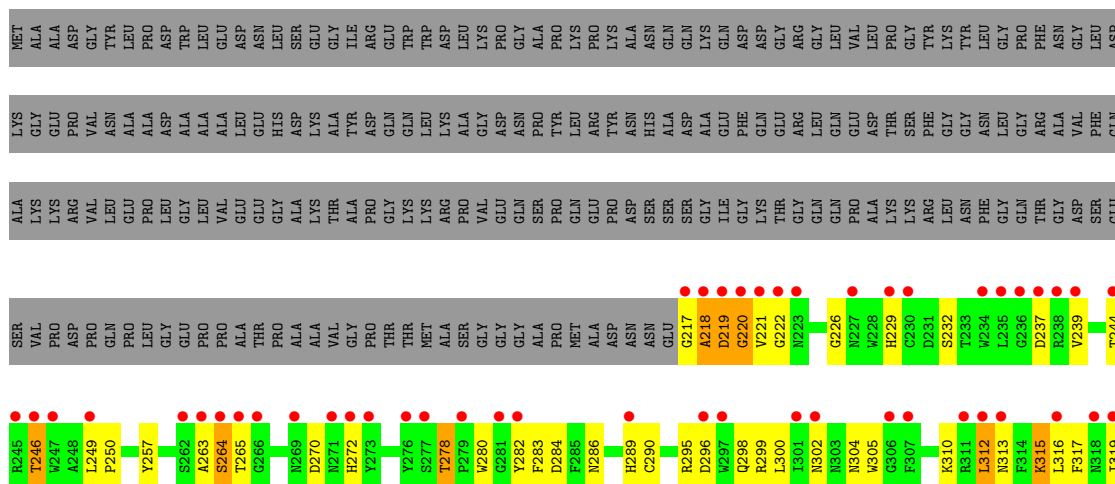
● Molecule 1: Capsid protein

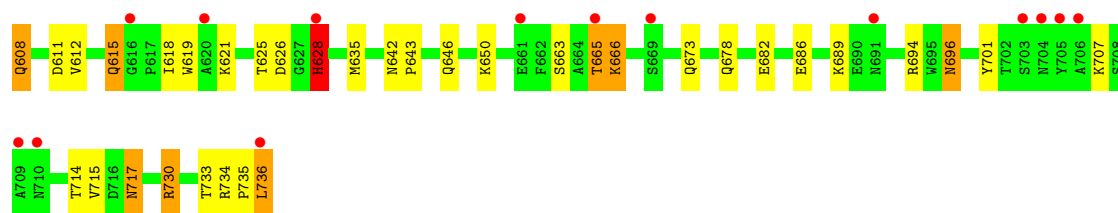




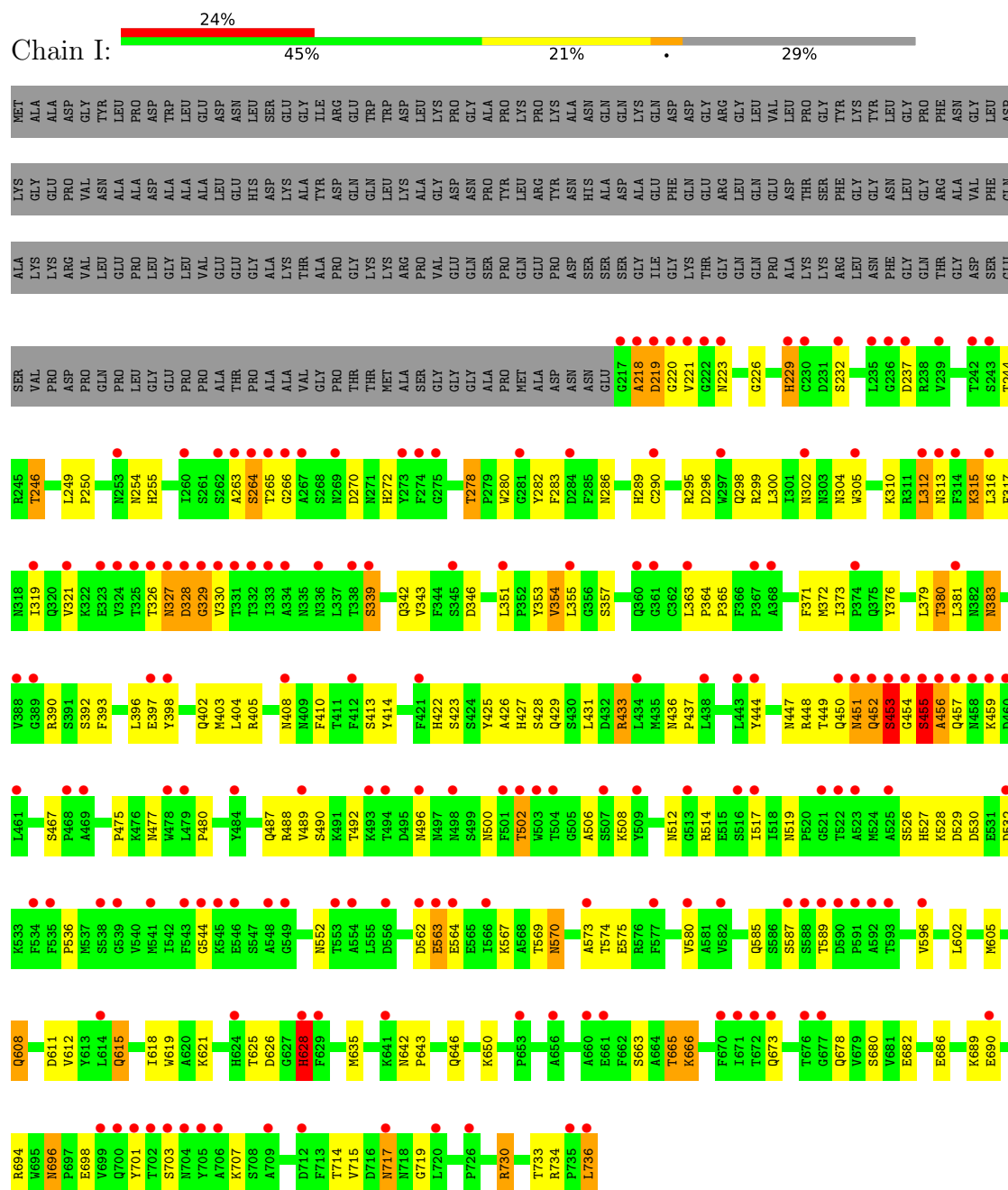


- Molecule 1: Capsid protein





● Molecule 1: Capsid protein



● Molecule 1: Capsid protein



ALA	LYS	ALA	SER	S243	L312	G377	L438	S507	V572	Q646	D712
LYS	GLY	ALA	VAL	T244	N313	Y376	I439	K508	A573	I647	F713
GLU	PRO	LYS	PRO	R245	F314	L379	L443	N509	T574	K650	T714
VAL	VAL	ARG	ASP	T246	K315	T380	Y444	N510	E575	G651	V715
LEU	ASN	GLN	PRO	W247	L316	L381	G445	N511	R576	N651	D716
ALA	ALA	LEU	PRO	A248	F317	N382	W447	N512	F577	P652	N717
PRO	GLU	PRO	PRO	L249	N318	N383	R448	R514	G578	G653	N718
ASP	ALA	LEU	LEU	P250	I319	G384	T449	G514	T579	V654	G719
LEU	ASP	GLY	GLY	N253	G320	S385	Q450	I517	V580	P655	L720
ALA	ALA	GLY	GLU	N254	V321	S386	Q451	I518	S587	A656	Y721
VAL	ALA	LEU	PRO	H255	K322	A387	N451	N519	S588	N657	P724
GLU	VAL	VAL	PRO	L256	E323	V388	Q452	P520	T589	P658	R725
ASN	GLU	GLU	ALA	Y257	V324	G389	S453	P521	D590	P659	P726
LEU	GLU	LEU	THR		T325	K390	G454	G521	G591	A660	L727
HIS	HIS	GLY	PRO		T326	S391	S455	M524	A592	F661	
ASP	ASP	ALA	ALA	I260	N327	S392	A456	S525	A593	F662	
LYS	LYS	ALA	VAL	S261	D328	F393	Q457	S526	T593	S663	R730
GLY	THR	THR	VAL	S262	G329	Y394	N458	S527	G594	A664	Y731
TLE	ALA	ALA	GLY	A263	V330	C395	K459	H527	D595	T665	L732
ARG	PRO	PRO	PRO	S264	T331	L396	D460	K528	V596	K666	T733
GLN	GLY	GLY	THR	G266	T332	E397	L461	D529	H597	P667	R734
TRP	GLN	LYS	THR	G267	I333	Y398	L462	D530	A598	A668	R735
LEU	LEU	LYS	MET	A267	A334	F399	F463	E531	N599	S669	
ASP	LYS	ARG	ALA	S268	N335	P400	S464	D532	G600	F670	
LEU	PRO	LEU	VAL	N269	N336	S401	R465	K533	A601	L671	
GLY	ALA	VAL	GLY	D270	L337	Q402	G466	F534	L602	T672	
ASP	GLU	GLN	GLY	N271	T338	M403	S467	F535	M605	Q673	
ASN	ASN	GLN	GLY	H272	S339	L404	P468	P536	V606	T676	
PRO	PRO	PRO	ALA	Y273		R405	A469	G539	W607	G677	
LYS	LEU	GLN	MET		Q342	T406		V540	O608	G678	
PRO	ARG	PRO	GLU	S277	V343	Q407	K476	M541	D611	V679	
LYS	TYR	PRO	GLU	T278	F344	M408	N477	I542	W612	S680	
ASN	ASN	ASP	ASP	G281	S345	N409	W478	F543	V613	V681	
ALA	HIS	SER	SER	W280	D346	F410	L479	G544	L614	E682	
GLN	ALA	SER	GLU	Y282	S347	T411	P480	K545	Q615	E686	
ASP	ASP	SER	SER	F283	G350	S413	G481	E546	G616	L687	
ALA	ALA	GLY	GLY	D284	L351	Y414	C483	S547	P617	Q688	
GLN	GLU	TLE	GLU	F285	F352	T415	Q486	A548	T618	K689	
ASP	PHE	GLY	GLY	N286	Y353	F416	R487	G549	W619	E690	
GLY	GLN	LYS	LYS		V354	E417	R488	A550	A620	N691	
ASP	GLU	THR	THR	H289	L355	E418	V489	N551	K621	S692	
ARG	ARG	GLY	GLY	C290	G356	E421	S490	N552	T622	K693	
GLY	LEU	GLN	GLN		S357	H422	K491	A554	P623		
LEU	GLU	PRO	GLN	R295	A358	S428	T492	L555	H624		
VAL	ASP	ALA	ALA	D296	H359	S423	K493	D556	T625		
THR	THR	LYS	LYS	W297	Q360	S424	T494	N557	D626		
PRO	PRO	LYS	LYS	Q298	L363	A426	D495		G627		
GLY	SER	LYS	ARG	R299	P364	H427	N496	T561	H628		
TYR	PHE	ARG	LEU	L300	F365	S428	N497	D562			
LYS	GLY	LEU	LEU	I301	F366	Q429	N498	E563	P631		
TYR	GLY	ASN	GLY	N302	P367	S430	S499	E564	S632		
LYS	ASN	PHE	PHE	N303		L431	N500	E565			
LEU	GLY	GLY	GLY	N304		D432	F501	I566	L640		
PRO	GLY	GLN	GLY	W305		R433	T502	K567	K641		
ARG	ARG	THR	THR	G306		L434	W503	A568	N642		
PHE	GLY	GLY	GLY	F307		P374	T504	I569	P643		
ASN	ALA	ASP	ASP	V239		Q375	G505	N570	P644		
GLY	PHE	LEU	LEU	T241		Y376	A506	P571	P645		
LEU	GLN	ASP	GLU	T242							

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	262.70Å 262.70Å 612.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-2.50) 89.0 (50.00-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.250 0.257 , 0.261	Depositor DCC
R_{free} test set	12421 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.009 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.017 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	42680	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADE, CYT

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	0.94	0/4246	1.04	11/5790 (0.2%)
1	B	0.94	0/4246	1.05	14/5790 (0.2%)
1	C	0.95	0/4246	1.04	10/5790 (0.2%)
1	D	0.94	0/4246	1.04	10/5790 (0.2%)
1	E	0.94	0/4246	1.05	12/5790 (0.2%)
1	F	0.93	0/4246	1.02	8/5790 (0.1%)
1	G	0.93	0/4246	1.04	12/5790 (0.2%)
1	H	0.95	0/4246	1.05	12/5790 (0.2%)
1	I	0.93	0/4246	1.03	10/5790 (0.2%)
1	J	0.94	0/4246	1.03	10/5790 (0.2%)
All	All	0.94	0/42460	1.04	109/57900 (0.2%)

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	8
1	B	0	8
1	C	0	8
1	D	0	7
1	E	0	5
1	F	0	8
1	G	0	6
1	H	0	6
1	I	0	10
1	J	0	6
All	All	0	72

There are no bond length outliers.

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ASN	CA-C-N	-6.18	113.44	122.65
1	B	327	ASN	C-N-CA	-6.18	113.44	122.65
1	B	399	PHE	CA-C-N	-5.81	113.56	119.83
1	B	399	PHE	C-N-CA	-5.81	113.56	119.83
1	H	399	PHE	CA-C-N	-5.80	113.56	119.83
1	H	399	PHE	C-N-CA	-5.80	113.56	119.83
1	G	399	PHE	CA-C-N	-5.79	113.58	119.83
1	G	399	PHE	C-N-CA	-5.79	113.58	119.83
1	E	399	PHE	CA-C-N	-5.78	113.58	119.83
1	E	399	PHE	C-N-CA	-5.78	113.58	119.83
1	D	264	SER	CB-CA-C	-5.73	109.99	116.63
1	J	264	SER	CB-CA-C	-5.69	110.03	116.63
1	G	264	SER	CB-CA-C	-5.67	110.05	116.63
1	H	264	SER	CB-CA-C	-5.66	110.06	116.63
1	A	264	SER	CB-CA-C	-5.64	110.09	116.63
1	I	264	SER	CB-CA-C	-5.61	110.12	116.63
1	C	264	SER	CB-CA-C	-5.59	110.15	116.63
1	A	328	ASP	CB-CA-C	-5.58	110.16	116.63
1	C	300	LEU	N-CA-C	-5.56	105.14	111.14
1	J	300	LEU	N-CA-C	-5.56	105.14	111.14
1	H	300	LEU	N-CA-C	-5.55	105.15	111.14
1	D	642	ASN	CA-C-N	5.55	126.09	120.38
1	D	642	ASN	C-N-CA	5.55	126.09	120.38
1	E	300	LEU	N-CA-C	-5.54	105.15	111.14
1	G	642	ASN	CA-C-N	5.54	126.09	120.38
1	G	642	ASN	C-N-CA	5.54	126.09	120.38
1	A	300	LEU	N-CA-C	-5.54	105.16	111.14
1	E	642	ASN	CA-C-N	5.54	126.08	120.38
1	E	642	ASN	C-N-CA	5.54	126.08	120.38
1	G	300	LEU	N-CA-C	-5.54	105.16	111.14
1	D	300	LEU	N-CA-C	-5.52	105.18	111.14
1	I	300	LEU	N-CA-C	-5.50	105.20	111.14
1	H	642	ASN	CA-C-N	5.50	126.04	120.38
1	H	642	ASN	C-N-CA	5.50	126.04	120.38
1	B	300	LEU	N-CA-C	-5.50	105.20	111.14
1	A	642	ASN	CA-C-N	5.49	126.04	120.38
1	A	642	ASN	C-N-CA	5.49	126.04	120.38
1	J	642	ASN	CA-C-N	5.48	126.02	120.38
1	J	642	ASN	C-N-CA	5.48	126.02	120.38
1	C	642	ASN	CA-C-N	5.47	126.02	120.38
1	C	642	ASN	C-N-CA	5.47	126.02	120.38
1	I	642	ASN	CA-C-N	5.47	126.01	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	642	ASN	C-N-CA	5.47	126.01	120.38
1	F	642	ASN	CA-C-N	5.45	125.99	120.38
1	F	642	ASN	C-N-CA	5.45	125.99	120.38
1	B	642	ASN	CA-C-N	5.44	125.98	120.38
1	B	642	ASN	C-N-CA	5.44	125.98	120.38
1	F	290	CYS	N-CA-C	-5.41	106.18	112.89
1	I	290	CYS	N-CA-C	-5.40	106.20	112.89
1	C	290	CYS	N-CA-C	-5.39	106.20	112.89
1	J	290	CYS	N-CA-C	-5.38	106.21	112.89
1	A	290	CYS	N-CA-C	-5.37	106.23	112.89
1	B	290	CYS	N-CA-C	-5.37	106.23	112.89
1	H	290	CYS	N-CA-C	-5.37	106.23	112.89
1	G	290	CYS	N-CA-C	-5.36	106.25	112.89
1	D	290	CYS	N-CA-C	-5.35	106.26	112.89
1	E	290	CYS	N-CA-C	-5.33	106.28	112.89
1	B	264	SER	CB-CA-C	-5.28	110.05	117.23
1	G	526	SER	N-CA-C	5.24	117.73	111.71
1	B	502	THR	N-CA-C	5.22	116.65	111.07
1	D	526	SER	N-CA-C	5.22	117.71	111.71
1	E	269	ASN	N-CA-C	-5.21	105.72	111.71
1	F	526	SER	N-CA-C	5.20	117.69	111.71
1	E	526	SER	N-CA-C	5.20	117.69	111.71
1	A	526	SER	N-CA-C	5.20	117.68	111.71
1	E	502	THR	N-CA-C	5.19	116.62	111.07
1	B	526	SER	N-CA-C	5.19	117.68	111.71
1	C	526	SER	N-CA-C	5.19	117.67	111.71
1	I	526	SER	N-CA-C	5.19	117.67	111.71
1	H	526	SER	N-CA-C	5.17	117.66	111.71
1	J	526	SER	N-CA-C	5.17	117.66	111.71
1	D	628	HIS	N-CA-C	-5.17	101.56	109.41
1	H	673	GLN	N-CA-C	5.16	116.65	108.96
1	B	673	GLN	N-CA-C	5.16	116.65	108.96
1	D	502	THR	N-CA-C	5.16	116.59	111.07
1	F	628	HIS	N-CA-C	-5.16	101.57	109.41
1	C	502	THR	N-CA-C	5.16	116.59	111.07
1	G	673	GLN	N-CA-C	5.16	116.65	108.96
1	H	502	THR	N-CA-C	5.16	116.59	111.07
1	A	502	THR	N-CA-C	5.16	116.59	111.07
1	E	673	GLN	N-CA-C	5.16	116.64	108.96
1	A	628	HIS	N-CA-C	-5.15	101.58	109.41
1	E	628	HIS	N-CA-C	-5.15	101.58	109.41
1	F	502	THR	N-CA-C	5.14	116.58	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	502	THR	N-CA-C	5.14	116.58	111.07
1	I	628	HIS	N-CA-C	-5.14	101.59	109.41
1	A	673	GLN	N-CA-C	5.14	116.62	108.96
1	D	673	GLN	N-CA-C	5.14	116.62	108.96
1	H	628	HIS	N-CA-C	-5.14	101.60	109.41
1	C	628	HIS	N-CA-C	-5.14	101.60	109.41
1	C	673	GLN	N-CA-C	5.14	116.61	108.96
1	F	673	GLN	N-CA-C	5.14	116.61	108.96
1	B	628	HIS	N-CA-C	-5.13	101.61	109.41
1	G	628	HIS	N-CA-C	-5.13	101.61	109.41
1	I	673	GLN	N-CA-C	5.13	116.61	108.96
1	J	628	HIS	N-CA-C	-5.13	101.61	109.41
1	J	673	GLN	N-CA-C	5.13	116.60	108.96
1	J	502	THR	N-CA-C	5.13	116.56	111.07
1	G	502	THR	N-CA-C	5.12	116.55	111.07
1	H	730	ARG	N-CA-C	5.10	117.44	108.56
1	B	730	ARG	N-CA-C	5.09	117.42	108.56
1	F	730	ARG	N-CA-C	5.09	117.42	108.56
1	G	730	ARG	N-CA-C	5.09	117.41	108.56
1	A	730	ARG	N-CA-C	5.08	117.39	108.56
1	D	730	ARG	N-CA-C	5.07	117.39	108.56
1	I	730	ARG	N-CA-C	5.07	117.39	108.56
1	E	730	ARG	N-CA-C	5.06	117.37	108.56
1	J	730	ARG	N-CA-C	5.06	117.37	108.56
1	C	730	ARG	N-CA-C	5.06	117.36	108.56

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	GLY	Peptide
1	A	219	ASP	Peptide
1	A	263	ALA	Peptide
1	A	328	ASP	Peptide
1	A	329	GLY	Peptide
1	A	451	ASN	Peptide
1	A	453	SER	Peptide
1	A	454	GLY	Peptide
1	B	218	ALA	Peptide
1	B	219	ASP	Peptide
1	B	220	GLY	Peptide
1	B	326	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	329	GLY	Peptide
1	B	330	VAL	Peptide
1	B	451	ASN	Peptide
1	B	453	SER	Peptide
1	C	217	GLY	Peptide
1	C	219	ASP	Peptide
1	C	220	GLY	Peptide
1	C	328	ASP	Peptide
1	C	329	GLY	Peptide
1	C	398	TYR	Peptide
1	C	451	ASN	Peptide
1	C	453	SER	Peptide
1	D	219	ASP	Peptide
1	D	220	GLY	Peptide
1	D	263	ALA	Peptide
1	D	327	ASN	Peptide
1	D	328	ASP	Peptide
1	D	451	ASN	Peptide
1	D	453	SER	Peptide
1	E	218	ALA	Peptide
1	E	219	ASP	Peptide
1	E	220	GLY	Peptide
1	E	451	ASN	Peptide
1	E	453	SER	Peptide
1	F	219	ASP	Peptide
1	F	220	GLY	Peptide
1	F	326	THR	Peptide
1	F	327	ASN	Peptide
1	F	328	ASP	Peptide
1	F	329	GLY	Peptide
1	F	451	ASN	Peptide
1	F	453	SER	Peptide
1	G	218	ALA	Peptide
1	G	220	GLY	Peptide
1	G	328	ASP	Peptide
1	G	329	GLY	Peptide
1	G	451	ASN	Peptide
1	G	453	SER	Peptide
1	H	219	ASP	Peptide
1	H	220	GLY	Peptide
1	H	328	ASP	Peptide
1	H	329	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	H	451	ASN	Peptide
1	H	453	SER	Peptide
1	I	218	ALA	Peptide
1	I	220	GLY	Peptide
1	I	326	THR	Peptide
1	I	327	ASN	Peptide
1	I	328	ASP	Peptide
1	I	329	GLY	Peptide
1	I	451	ASN	Peptide
1	I	453	SER	Peptide
1	I	455	SER	Peptide
1	I	456	ALA	Peptide
1	J	217	GLY	Peptide
1	J	218	ALA	Peptide
1	J	328	ASP	Peptide
1	J	398	TYR	Peptide
1	J	451	ASN	Peptide
1	J	453	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4120	0	3884	207	0
1	B	4120	0	3884	196	0
1	C	4120	0	3884	177	0
1	D	4120	0	3884	194	0
1	E	4120	0	3884	189	0
1	F	4120	0	3884	196	0
1	G	4120	0	3884	197	0
1	H	4120	0	3884	192	0
1	I	4120	0	3884	211	0
1	J	4120	0	3884	130	0
2	A	10	0	4	0	0
2	B	10	0	4	3	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	10	0	4	0	0
2	G	10	0	4	0	0
2	H	10	0	4	0	0
2	I	10	0	4	0	0
2	J	10	0	4	0	0
3	A	8	0	4	3	0
3	B	16	0	8	1	0
3	C	8	0	4	3	0
3	D	8	0	4	3	0
3	E	8	0	4	1	0
3	F	8	0	4	2	0
3	H	8	0	4	3	0
3	I	8	0	4	2	0
3	J	8	0	4	1	0
4	A	131	0	0	6	0
4	B	130	0	0	7	0
4	C	128	0	0	4	0
4	D	131	0	0	9	0
4	E	133	0	0	9	0
4	F	131	0	0	4	0
4	G	127	0	0	7	0
4	H	130	0	0	5	0
4	I	130	0	0	6	0
4	J	129	0	0	5	0
All	All	42680	0	38920	1620	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1620) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:328:ASP:HB3	1:G:329:GLY:C	1.41	1.45
1:C:328:ASP:HB3	1:C:329:GLY:C	1.41	1.44
1:H:328:ASP:HB3	1:H:329:GLY:C	1.41	1.42
1:D:328:ASP:CB	1:D:329:GLY:HA3	1.42	1.29
1:B:328:ASP:OD1	1:B:329:GLY:HA2	1.28	1.28
1:B:451:ASN:HA	1:B:452:GLN:HB2	1.17	1.16
1:E:451:ASN:HA	1:E:452:GLN:HB2	1.17	1.15
1:A:451:ASN:HB2	1:A:452:GLN:HB3	1.29	1.15
1:H:451:ASN:HA	1:H:452:GLN:HB2	1.17	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:ASP:HB3	1:D:329:GLY:HA3	1.21	1.14
1:I:397:GLU:OE1	1:I:650:LYS:HE2	1.42	1.14
1:D:328:ASP:HB2	1:D:329:GLY:HA3	1.14	1.12
1:J:451:ASN:HA	1:J:452:GLN:HB2	1.17	1.12
1:D:328:ASP:CB	1:D:329:GLY:CA	2.29	1.10
1:D:451:ASN:HA	1:D:452:GLN:HB2	1.17	1.10
1:G:451:ASN:HA	1:G:452:GLN:HB2	1.17	1.10
1:F:451:ASN:CB	1:F:452:GLN:HB3	1.83	1.08
1:C:451:ASN:HA	1:C:452:GLN:HB2	1.18	1.08
1:A:330:VAL:HG11	1:B:327:ASN:OD1	1.55	1.06
1:A:502:THR:O	1:A:506:ALA:HB2	1.55	1.06
1:C:502:THR:O	1:C:506:ALA:HB2	1.55	1.06
1:F:502:THR:O	1:F:506:ALA:HB2	1.55	1.06
1:J:380:THR:HG21	1:J:392:SER:H	1.06	1.06
1:C:380:THR:HG23	4:C:843:HOH:O	1.54	1.05
1:F:451:ASN:HA	1:F:452:GLN:CB	1.85	1.05
1:G:380:THR:HG21	1:G:392:SER:H	1.21	1.05
1:B:380:THR:HG21	1:B:392:SER:H	1.21	1.05
1:B:502:THR:O	1:B:506:ALA:HB2	1.55	1.05
1:I:502:THR:O	1:I:506:ALA:HB2	1.55	1.05
1:J:502:THR:O	1:J:506:ALA:HB2	1.56	1.04
1:B:663:SER:OG	1:B:665:THR:HG23	1.58	1.04
1:G:502:THR:O	1:G:506:ALA:HB2	1.55	1.04
1:H:502:THR:O	1:H:506:ALA:HB2	1.55	1.04
1:I:380:THR:HG21	1:I:392:SER:H	1.21	1.04
1:H:328:ASP:CB	1:H:329:GLY:C	2.32	1.03
1:B:328:ASP:OD1	1:B:329:GLY:CA	2.05	1.03
1:D:502:THR:O	1:D:506:ALA:HB2	1.55	1.03
1:G:328:ASP:HB3	1:G:329:GLY:CA	1.88	1.03
1:E:380:THR:HG21	1:E:392:SER:H	1.21	1.02
1:E:502:THR:O	1:E:506:ALA:HB2	1.56	1.02
1:A:380:THR:HG21	1:A:392:SER:H	1.21	1.02
1:B:326:THR:HG22	1:B:327:ASN:O	1.58	1.02
1:C:328:ASP:HB3	1:C:329:GLY:CA	1.88	1.02
1:F:380:THR:HG21	1:F:392:SER:H	1.21	1.01
1:G:328:ASP:CB	1:G:329:GLY:C	2.31	1.01
1:C:328:ASP:CB	1:C:329:GLY:C	2.32	1.01
1:C:380:THR:HG21	1:C:392:SER:H	1.21	1.01
1:D:380:THR:HG21	1:D:392:SER:H	1.21	1.01
1:I:451:ASN:HB2	1:I:452:GLN:HB3	1.38	1.00
1:D:393:PHE:H	1:H:696:ASN:HD21	1.09	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:380:THR:HG21	1:H:392:SER:H	1.21	1.00
1:B:312:LEU:C	1:B:312:LEU:HD23	1.88	0.99
1:A:312:LEU:HD23	1:A:312:LEU:C	1.88	0.99
1:C:393:PHE:H	1:F:696:ASN:HD21	1.10	0.99
1:J:312:LEU:C	1:J:312:LEU:HD23	1.88	0.99
1:D:312:LEU:C	1:D:312:LEU:HD23	1.87	0.99
1:I:312:LEU:C	1:I:312:LEU:HD23	1.88	0.99
1:F:312:LEU:HD23	1:F:312:LEU:C	1.88	0.99
1:C:312:LEU:HD23	1:C:312:LEU:C	1.88	0.98
1:H:328:ASP:HB3	1:H:329:GLY:CA	1.88	0.98
1:H:312:LEU:HD23	1:H:312:LEU:C	1.88	0.98
1:C:696:ASN:HD21	1:I:393:PHE:H	1.12	0.98
1:E:312:LEU:C	1:E:312:LEU:HD23	1.88	0.98
1:G:312:LEU:C	1:G:312:LEU:HD23	1.88	0.97
1:A:451:ASN:CB	1:A:452:GLN:HB3	1.94	0.96
1:B:269:ASN:HA	1:B:272:HIS:HD2	1.31	0.96
1:H:451:ASN:CA	1:H:452:GLN:HB2	1.96	0.96
1:D:451:ASN:CA	1:D:452:GLN:HB2	1.96	0.96
1:E:278:THR:HG22	1:E:280:TRP:H	1.31	0.96
1:D:328:ASP:HB2	1:D:329:GLY:CA	1.95	0.95
1:F:451:ASN:HA	1:F:452:GLN:HB2	1.44	0.95
1:A:393:PHE:H	1:D:696:ASN:HD21	1.10	0.95
1:B:278:THR:HG22	1:B:280:TRP:H	1.31	0.95
1:I:278:THR:HG22	1:I:280:TRP:H	1.31	0.95
1:C:278:THR:HG22	1:C:280:TRP:H	1.31	0.95
1:G:278:THR:HG22	1:G:280:TRP:H	1.31	0.95
1:A:696:ASN:HD21	1:H:393:PHE:H	1.10	0.95
1:F:278:THR:HG22	1:F:280:TRP:H	1.31	0.94
1:B:451:ASN:CA	1:B:452:GLN:HB2	1.96	0.94
1:G:451:ASN:CA	1:G:452:GLN:HB2	1.96	0.94
1:E:451:ASN:CA	1:E:452:GLN:HB2	1.96	0.94
1:E:663:SER:OG	1:E:665:THR:HG23	1.65	0.94
1:F:451:ASN:CA	1:F:452:GLN:HB3	1.96	0.94
1:C:451:ASN:CA	1:C:452:GLN:HB2	1.98	0.94
1:D:278:THR:HG22	1:D:280:TRP:H	1.31	0.94
1:J:451:ASN:CA	1:J:452:GLN:HB2	1.96	0.94
1:J:278:THR:HG22	1:J:280:TRP:H	1.31	0.93
1:F:393:PHE:H	1:I:696:ASN:HD21	1.09	0.93
1:B:393:PHE:H	1:E:696:ASN:HD21	1.10	0.93
1:F:451:ASN:CA	1:F:452:GLN:CB	2.47	0.92
1:H:278:THR:HG22	1:H:280:TRP:H	1.31	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:328:ASP:HA	1:I:329:GLY:C	1.92	0.92
1:J:327:ASN:O	1:J:328:ASP:HB2	1.67	0.92
1:A:278:THR:HG22	1:A:280:TRP:H	1.31	0.92
1:J:218:ALA:HB3	1:J:407:GLY:O	1.69	0.92
1:B:696:ASN:HD21	1:G:393:PHE:H	1.11	0.91
1:E:393:PHE:H	1:G:696:ASN:HD21	1.10	0.91
1:G:239:VAL:CG1	1:G:685:TRP:HB2	2.01	0.91
1:G:328:ASP:HB3	1:G:329:GLY:O	1.71	0.90
1:E:328:ASP:HA	1:E:329:GLY:C	1.96	0.90
1:D:328:ASP:HB3	1:D:329:GLY:CA	1.99	0.90
1:J:312:LEU:HD22	1:J:414:TYR:HB3	1.53	0.90
1:B:312:LEU:HD22	1:B:414:TYR:HB3	1.53	0.90
1:D:312:LEU:HD22	1:D:414:TYR:HB3	1.53	0.90
1:F:312:LEU:HD22	1:F:414:TYR:HB3	1.53	0.90
1:I:451:ASN:CB	1:I:452:GLN:HB3	2.02	0.90
1:B:326:THR:CG2	1:B:327:ASN:O	2.19	0.90
1:F:456:ALA:C	1:F:457:GLN:OE1	2.15	0.89
1:G:312:LEU:HD22	1:G:414:TYR:HB3	1.53	0.89
1:A:451:ASN:HA	1:A:452:GLN:HB2	1.53	0.89
1:C:328:ASP:HB3	1:C:329:GLY:O	1.71	0.89
1:A:328:ASP:OD1	1:A:329:GLY:CA	2.21	0.88
1:D:246:THR:HB	1:D:678:GLN:HE21	1.39	0.88
1:C:312:LEU:HD22	1:C:414:TYR:HB3	1.53	0.88
1:I:280:TRP:CE2	1:I:650:LYS:HD3	2.08	0.88
1:A:312:LEU:HD22	1:A:414:TYR:HB3	1.53	0.88
1:B:246:THR:HB	1:B:678:GLN:HE21	1.39	0.88
1:H:328:ASP:HB3	1:H:329:GLY:O	1.71	0.88
1:A:328:ASP:CG	1:A:329:GLY:N	2.30	0.88
1:C:246:THR:HB	1:C:678:GLN:HE21	1.39	0.88
1:E:312:LEU:HD22	1:E:414:TYR:HB3	1.53	0.88
1:F:246:THR:HB	1:F:678:GLN:HE21	1.39	0.88
1:I:312:LEU:HD22	1:I:414:TYR:HB3	1.53	0.88
1:J:451:ASN:HA	1:J:452:GLN:CB	2.04	0.88
1:E:246:THR:HB	1:E:678:GLN:HE21	1.39	0.87
1:H:246:THR:HB	1:H:678:GLN:HE21	1.39	0.87
1:G:246:THR:HB	1:G:678:GLN:HE21	1.39	0.87
1:H:312:LEU:HD22	1:H:414:TYR:HB3	1.53	0.86
1:H:451:ASN:HA	1:H:452:GLN:CB	2.04	0.86
1:H:570:ASN:HD21	1:H:608:GLN:H	1.24	0.86
1:B:451:ASN:HA	1:B:452:GLN:CB	2.04	0.86
1:J:246:THR:HB	1:J:678:GLN:HE21	1.39	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:452:GLN:O	1:I:454:GLY:HA3	1.75	0.86
1:D:451:ASN:HA	1:D:452:GLN:CB	2.03	0.86
1:G:451:ASN:HA	1:G:452:GLN:CB	2.04	0.86
1:A:696:ASN:ND2	1:H:393:PHE:H	1.75	0.85
1:D:393:PHE:H	1:H:696:ASN:ND2	1.74	0.85
1:A:393:PHE:H	1:D:696:ASN:ND2	1.75	0.85
1:E:451:ASN:HA	1:E:452:GLN:CB	2.04	0.85
1:F:393:PHE:H	1:I:696:ASN:ND2	1.74	0.85
1:I:246:THR:HB	1:I:678:GLN:HE21	1.39	0.84
1:A:246:THR:HB	1:A:678:GLN:HE21	1.39	0.84
1:B:393:PHE:H	1:E:696:ASN:ND2	1.74	0.84
1:B:696:ASN:ND2	1:G:393:PHE:H	1.75	0.84
1:B:269:ASN:HA	1:B:272:HIS:CD2	2.13	0.84
1:I:570:ASN:HD21	1:I:608:GLN:H	1.24	0.84
1:E:393:PHE:H	1:G:696:ASN:ND2	1.75	0.84
1:G:570:ASN:HD21	1:G:608:GLN:H	1.24	0.84
1:J:570:ASN:HD21	1:J:608:GLN:H	1.24	0.84
1:A:570:ASN:HD21	1:A:608:GLN:H	1.24	0.84
1:B:570:ASN:HD21	1:B:608:GLN:H	1.24	0.84
1:C:451:ASN:HA	1:C:452:GLN:CB	2.04	0.84
1:G:327:ASN:O	1:G:328:ASP:HB2	1.77	0.84
1:C:393:PHE:H	1:F:696:ASN:ND2	1.75	0.83
1:C:570:ASN:HD21	1:C:608:GLN:H	1.24	0.83
1:F:451:ASN:HB2	1:F:452:GLN:HB3	1.59	0.83
1:E:570:ASN:HD21	1:E:608:GLN:H	1.24	0.83
1:A:328:ASP:OD1	1:A:329:GLY:HA3	1.77	0.83
1:H:327:ASN:O	1:H:328:ASP:HB2	1.77	0.83
1:A:451:ASN:HA	1:A:452:GLN:CB	2.09	0.83
1:C:585:GLN:HE22	1:I:496:ASN:HD22	1.27	0.83
1:C:696:ASN:ND2	1:I:393:PHE:H	1.75	0.83
1:A:585:GLN:HE22	1:H:496:ASN:HD22	1.27	0.83
1:F:570:ASN:HD21	1:F:608:GLN:H	1.24	0.83
1:C:327:ASN:O	1:C:328:ASP:HB2	1.77	0.82
1:D:496:ASN:HD22	1:H:585:GLN:HE22	1.27	0.82
1:B:496:ASN:HD22	1:E:585:GLN:HE22	1.27	0.82
1:A:496:ASN:HD22	1:D:585:GLN:HE22	1.27	0.82
1:B:512:ASN:HD21	1:E:529:ASP:H	1.28	0.81
1:D:512:ASN:HD21	1:H:529:ASP:H	1.28	0.81
1:D:570:ASN:HD21	1:D:608:GLN:H	1.24	0.81
1:B:328:ASP:HA	1:B:329:GLY:C	2.04	0.81
1:C:496:ASN:HD22	1:F:585:GLN:HE22	1.27	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:THR:HG22	1:D:715:VAL:N	1.96	0.81
1:I:451:ASN:HA	1:I:452:GLN:HB2	1.61	0.81
1:B:585:GLN:HE22	1:G:496:ASN:HD22	1.28	0.81
1:B:490:SER:H	1:B:496:ASN:HD21	1.29	0.80
1:A:451:ASN:CA	1:A:452:GLN:CB	2.60	0.80
1:J:380:THR:HG21	1:J:392:SER:N	1.91	0.80
1:A:490:SER:H	1:A:496:ASN:HD21	1.29	0.80
1:G:237:ASP:O	1:G:687:LEU:HG	1.80	0.80
1:C:490:SER:H	1:C:496:ASN:HD21	1.29	0.80
1:C:512:ASN:HD21	1:F:529:ASP:H	1.29	0.80
1:C:529:ASP:H	1:I:512:ASN:HD21	1.26	0.80
1:H:490:SER:H	1:H:496:ASN:HD21	1.29	0.80
1:E:496:ASN:HD22	1:G:585:GLN:HE22	1.27	0.80
1:F:512:ASN:HD21	1:I:529:ASP:H	1.29	0.80
1:J:490:SER:H	1:J:496:ASN:HD21	1.29	0.79
1:I:451:ASN:HA	1:I:452:GLN:CB	2.12	0.79
1:I:453:SER:HA	1:I:455:SER:H	1.45	0.79
1:A:457:GLN:NE2	1:A:457:GLN:N	2.30	0.79
1:E:512:ASN:HD21	1:G:529:ASP:H	1.28	0.79
1:J:328:ASP:HB3	1:J:329:GLY:C	2.08	0.79
1:A:714:THR:HG22	1:A:715:VAL:N	1.96	0.79
1:C:696:ASN:HD22	1:C:696:ASN:H	1.30	0.79
1:E:490:SER:H	1:E:496:ASN:HD21	1.29	0.79
1:B:380:THR:HG23	4:B:842:HOH:O	1.82	0.79
1:A:328:ASP:CG	1:A:329:GLY:CA	2.55	0.79
1:F:496:ASN:HD22	1:I:585:GLN:HE22	1.27	0.79
1:C:714:THR:HG22	1:C:715:VAL:N	1.96	0.79
1:F:330:VAL:HG12	1:F:330:VAL:O	1.80	0.79
1:F:714:THR:HG22	1:F:715:VAL:N	1.96	0.79
1:B:714:THR:HG22	1:B:715:VAL:N	1.96	0.78
1:J:714:THR:HG22	1:J:715:VAL:N	1.96	0.78
1:E:696:ASN:H	1:E:696:ASN:HD22	1.30	0.78
1:A:512:ASN:HD21	1:D:529:ASP:H	1.29	0.78
1:A:529:ASP:H	1:H:512:ASN:HD21	1.29	0.78
1:E:714:THR:HG22	1:E:715:VAL:N	1.96	0.78
1:I:490:SER:H	1:I:496:ASN:HD21	1.29	0.78
1:B:696:ASN:H	1:B:696:ASN:HD22	1.30	0.78
1:I:714:THR:HG22	1:I:715:VAL:N	1.96	0.78
1:B:663:SER:HG	1:B:665:THR:HG23	1.49	0.78
1:F:490:SER:H	1:F:496:ASN:HD21	1.29	0.78
1:G:714:THR:HG22	1:G:715:VAL:N	1.96	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:SER:H	1:D:496:ASN:HD21	1.29	0.78
1:G:451:ASN:CA	1:G:452:GLN:CB	2.62	0.78
1:G:490:SER:H	1:G:496:ASN:HD21	1.29	0.78
1:B:218:ALA:HB1	1:B:219:ASP:OD1	1.83	0.77
1:F:696:ASN:HD22	1:F:696:ASN:H	1.30	0.77
1:B:529:ASP:H	1:G:512:ASN:HD21	1.29	0.77
1:A:696:ASN:HD22	1:A:696:ASN:H	1.30	0.77
1:B:451:ASN:CA	1:B:452:GLN:CB	2.62	0.77
1:H:714:THR:HG22	1:H:715:VAL:N	1.96	0.77
1:D:696:ASN:H	1:D:696:ASN:HD22	1.30	0.77
1:F:456:ALA:O	1:F:457:GLN:OE1	2.03	0.76
1:G:239:VAL:HG13	1:G:685:TRP:HB2	1.67	0.76
1:B:663:SER:OG	1:B:665:THR:CG2	2.34	0.76
1:G:696:ASN:H	1:G:696:ASN:HD22	1.30	0.76
1:H:696:ASN:HD22	1:H:696:ASN:H	1.30	0.76
1:I:696:ASN:H	1:I:696:ASN:HD22	1.30	0.76
1:J:451:ASN:CA	1:J:452:GLN:CB	2.62	0.75
1:J:696:ASN:HD22	1:J:696:ASN:H	1.32	0.75
1:D:380:THR:HG23	4:D:845:HOH:O	1.84	0.75
1:E:218:ALA:O	1:E:219:ASP:CG	2.30	0.75
1:F:218:ALA:O	1:F:219:ASP:CG	2.30	0.75
1:I:454:GLY:O	1:I:455:SER:CB	2.35	0.75
1:C:312:LEU:HD23	1:C:312:LEU:O	1.87	0.75
1:H:451:ASN:CA	1:H:452:GLN:CB	2.62	0.75
1:D:312:LEU:HD23	1:D:312:LEU:O	1.87	0.74
1:E:451:ASN:CA	1:E:452:GLN:CB	2.62	0.74
1:I:456:ALA:C	1:I:457:GLN:OE1	2.30	0.74
1:H:218:ALA:O	1:H:219:ASP:CG	2.30	0.74
1:A:218:ALA:O	1:A:219:ASP:CG	2.30	0.74
1:I:312:LEU:HD23	1:I:312:LEU:O	1.87	0.74
1:B:312:LEU:HD23	1:B:312:LEU:O	1.87	0.74
1:C:451:ASN:CA	1:C:452:GLN:CB	2.63	0.74
1:F:312:LEU:HD23	1:F:312:LEU:O	1.87	0.74
1:H:380:THR:HG21	1:H:392:SER:N	2.02	0.74
1:I:451:ASN:CA	1:I:452:GLN:CB	2.65	0.74
1:F:450:GLN:HB2	1:F:458:ASN:O	1.87	0.74
1:G:380:THR:HG23	4:G:845:HOH:O	1.88	0.74
1:G:312:LEU:HD23	1:G:312:LEU:O	1.87	0.74
1:J:380:THR:HG23	4:J:847:HOH:O	1.88	0.74
1:I:456:ALA:O	1:I:457:GLN:CD	2.30	0.73
1:I:663:SER:OG	1:I:665:THR:HG23	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:HIS:CD2	1:D:736:LEU:HD13	2.24	0.73
1:E:312:LEU:HD23	1:E:312:LEU:O	1.87	0.73
1:H:427:HIS:CD2	1:H:736:LEU:HD13	2.24	0.73
1:E:427:HIS:CD2	1:E:736:LEU:HD13	2.24	0.73
1:C:427:HIS:CD2	1:C:736:LEU:HD13	2.24	0.73
1:F:427:HIS:CD2	1:F:736:LEU:HD13	2.24	0.73
1:I:427:HIS:CD2	1:I:736:LEU:HD13	2.24	0.73
1:F:527:HIS:NE2	1:F:532:ASP:OD2	2.22	0.73
1:H:312:LEU:HD23	1:H:312:LEU:O	1.87	0.73
1:F:218:ALA:O	1:F:219:ASP:CB	2.36	0.73
1:H:218:ALA:O	1:H:219:ASP:CB	2.37	0.73
1:H:304:ASN:HD21	1:H:689:LYS:NZ	1.87	0.73
1:H:380:THR:HG23	4:H:845:HOH:O	1.88	0.73
1:J:427:HIS:CD2	1:J:736:LEU:HD13	2.24	0.73
1:C:451:ASN:HD21	1:C:458:ASN:HB2	1.54	0.73
1:G:527:HIS:NE2	1:G:532:ASP:OD2	2.22	0.73
1:J:312:LEU:HD23	1:J:312:LEU:O	1.87	0.73
1:E:527:HIS:NE2	1:E:532:ASP:OD2	2.22	0.73
1:B:380:THR:HG21	1:B:392:SER:N	2.02	0.72
1:G:239:VAL:HG12	1:G:685:TRP:HB2	1.69	0.72
1:J:527:HIS:NE2	1:J:532:ASP:OD2	2.22	0.72
1:C:304:ASN:HD21	1:C:689:LYS:NZ	1.87	0.72
1:D:527:HIS:NE2	1:D:532:ASP:OD2	2.22	0.72
1:E:380:THR:HG23	4:E:845:HOH:O	1.88	0.72
1:G:427:HIS:CD2	1:G:736:LEU:HD13	2.24	0.72
1:H:527:HIS:NE2	1:H:532:ASP:OD2	2.22	0.72
1:I:380:THR:HG23	4:I:847:HOH:O	1.88	0.72
1:C:527:HIS:NE2	1:C:532:ASP:OD2	2.22	0.72
1:J:304:ASN:HD21	1:J:689:LYS:NZ	1.87	0.72
1:A:304:ASN:HD21	1:A:689:LYS:NZ	1.87	0.72
1:B:527:HIS:NE2	1:B:532:ASP:OD2	2.22	0.72
1:D:304:ASN:HD21	1:D:689:LYS:NZ	1.87	0.72
1:F:380:THR:HG21	1:F:392:SER:N	2.02	0.72
1:B:427:HIS:CD2	1:B:736:LEU:HD13	2.24	0.72
1:A:217:GLY:HA3	1:A:408:ASN:HA	1.72	0.72
1:A:312:LEU:HD23	1:A:312:LEU:O	1.87	0.72
1:A:427:HIS:CD2	1:A:736:LEU:HD13	2.24	0.72
1:A:527:HIS:NE2	1:A:532:ASP:OD2	2.22	0.72
1:E:304:ASN:HD21	1:E:689:LYS:NZ	1.87	0.72
1:A:380:THR:HG23	4:A:842:HOH:O	1.88	0.72
1:I:304:ASN:HD21	1:I:689:LYS:NZ	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:ASN:HD21	1:G:689:LYS:NZ	1.87	0.71
1:I:527:HIS:NE2	1:I:532:ASP:OD2	2.22	0.71
1:A:451:ASN:CA	1:A:452:GLN:HB3	2.20	0.71
1:B:304:ASN:HD21	1:B:689:LYS:HZ1	1.36	0.71
1:I:380:THR:HG21	1:I:392:SER:N	2.02	0.71
1:A:457:GLN:N	1:A:457:GLN:HE21	1.87	0.71
1:B:304:ASN:HD21	1:B:689:LYS:NZ	1.87	0.71
1:A:328:ASP:CG	1:A:329:GLY:HA3	2.16	0.71
1:A:218:ALA:O	1:A:219:ASP:CB	2.38	0.71
1:G:383:ASN:C	1:G:383:ASN:HD22	1.99	0.71
1:B:383:ASN:C	1:B:383:ASN:HD22	1.99	0.70
1:C:380:THR:HG21	1:C:392:SER:N	2.02	0.70
1:I:453:SER:HA	1:I:455:SER:N	2.06	0.70
1:E:564:GLU:O	1:E:567:LYS:HG2	1.92	0.70
1:F:380:THR:HG23	4:F:844:HOH:O	1.88	0.70
1:I:383:ASN:C	1:I:383:ASN:HD22	1.99	0.70
1:J:564:GLU:O	1:J:567:LYS:HG2	1.92	0.70
1:A:383:ASN:C	1:A:383:ASN:HD22	1.99	0.70
1:I:564:GLU:O	1:I:567:LYS:HG2	1.92	0.70
1:F:383:ASN:C	1:F:383:ASN:HD22	1.99	0.70
1:A:457:GLN:HE21	1:A:457:GLN:H	1.39	0.70
1:E:380:THR:HG21	1:E:392:SER:N	2.02	0.70
1:E:383:ASN:C	1:E:383:ASN:HD22	1.99	0.70
1:F:217:GLY:HA3	1:F:408:ASN:HA	1.73	0.70
1:F:564:GLU:O	1:F:567:LYS:HG2	1.92	0.70
1:H:564:GLU:O	1:H:567:LYS:HG2	1.92	0.70
1:I:218:ALA:HB1	1:I:219:ASP:CG	2.17	0.70
1:C:383:ASN:C	1:C:383:ASN:HD22	1.99	0.69
1:J:383:ASN:C	1:J:383:ASN:HD22	1.99	0.69
1:A:564:GLU:O	1:A:567:LYS:HG2	1.92	0.69
1:D:451:ASN:CA	1:D:452:GLN:CB	2.62	0.69
1:F:714:THR:CG2	1:F:715:VAL:N	2.56	0.69
1:B:564:GLU:O	1:B:567:LYS:HG2	1.92	0.69
1:D:564:GLU:O	1:D:567:LYS:HG2	1.92	0.69
1:A:312:LEU:C	1:A:312:LEU:CD2	2.62	0.69
1:A:380:THR:HG22	1:D:428:SER:O	1.93	0.69
1:C:329:GLY:O	1:C:330:VAL:HG12	1.93	0.69
1:C:428:SER:O	1:I:380:THR:HG22	1.93	0.69
1:D:312:LEU:C	1:D:312:LEU:CD2	2.62	0.69
1:D:429:GLN:HE21	1:D:736:LEU:H	1.41	0.69
1:D:698:GLU:H	1:I:298:GLN:HE22	1.41	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:THR:CG2	1:D:715:VAL:N	2.56	0.69
1:F:429:GLN:HE21	1:F:736:LEU:H	1.41	0.69
1:I:451:ASN:CA	1:I:452:GLN:HB3	2.23	0.69
1:D:383:ASN:C	1:D:383:ASN:HD22	1.99	0.69
1:H:312:LEU:C	1:H:312:LEU:CD2	2.62	0.69
1:J:714:THR:CG2	1:J:715:VAL:N	2.56	0.69
1:H:383:ASN:C	1:H:383:ASN:HD22	1.99	0.69
1:F:380:THR:HG22	1:I:428:SER:O	1.93	0.68
1:H:329:GLY:O	1:H:330:VAL:HG12	1.93	0.68
1:A:428:SER:O	1:H:380:THR:HG22	1.92	0.68
1:B:380:THR:HG22	1:E:428:SER:O	1.93	0.68
1:C:564:GLU:O	1:C:567:LYS:HG2	1.92	0.68
1:H:714:THR:CG2	1:H:715:VAL:N	2.56	0.68
1:A:298:GLN:HE22	1:E:698:GLU:H	1.41	0.68
1:B:298:GLN:HE22	1:J:698:GLU:H	1.41	0.68
1:B:428:SER:O	1:G:380:THR:HG22	1.93	0.68
1:C:714:THR:CG2	1:C:715:VAL:N	2.56	0.68
1:D:298:GLN:HE22	1:I:698:GLU:H	1.41	0.68
1:G:217:GLY:HA2	1:G:408:ASN:HA	1.75	0.68
1:A:380:THR:HG21	1:A:392:SER:N	2.02	0.68
1:B:286:ASN:HD21	1:B:619:TRP:H	1.42	0.68
1:E:380:THR:HG22	1:G:428:SER:O	1.93	0.68
1:H:451:ASN:HD21	1:H:458:ASN:HB2	1.59	0.68
1:A:714:THR:CG2	1:A:715:VAL:N	2.56	0.68
1:D:286:ASN:HD21	1:D:619:TRP:H	1.42	0.68
1:I:714:THR:CG2	1:I:715:VAL:N	2.56	0.68
1:E:286:ASN:HD21	1:E:619:TRP:H	1.42	0.68
1:G:380:THR:HG21	1:G:392:SER:N	2.02	0.68
1:C:380:THR:HG22	1:F:428:SER:O	1.93	0.68
1:E:429:GLN:HE21	1:E:736:LEU:H	1.41	0.68
1:I:429:GLN:HE21	1:I:736:LEU:H	1.41	0.68
1:D:265:THR:HG21	1:D:267:ALA:HB2	1.74	0.68
1:E:714:THR:CG2	1:E:715:VAL:N	2.56	0.68
1:F:217:GLY:O	1:F:218:ALA:HB2	1.94	0.68
1:G:429:GLN:HE21	1:G:736:LEU:H	1.41	0.68
1:A:429:GLN:HE21	1:A:736:LEU:H	1.41	0.68
1:B:429:GLN:HE21	1:B:736:LEU:H	1.41	0.68
1:B:312:LEU:C	1:B:312:LEU:CD2	2.62	0.68
1:B:714:THR:CG2	1:B:715:VAL:N	2.56	0.68
1:C:286:ASN:HD21	1:C:619:TRP:H	1.42	0.68
1:D:278:THR:CG2	1:D:280:TRP:H	2.07	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:714:THR:CG2	1:G:715:VAL:N	2.56	0.68
1:G:451:ASN:HD21	1:G:458:ASN:HB2	1.59	0.67
1:J:310:LYS:HD2	1:J:686:GLU:HB2	1.77	0.67
1:J:304:ASN:HD21	1:J:689:LYS:HZ1	1.41	0.67
1:G:286:ASN:HD21	1:G:619:TRP:H	1.42	0.67
1:J:429:GLN:HE21	1:J:736:LEU:H	1.41	0.67
1:J:451:ASN:HD21	1:J:458:ASN:HB2	1.59	0.67
1:A:666:LYS:NZ	1:I:719:GLY:O	2.27	0.67
1:D:380:THR:HG21	1:D:392:SER:N	2.02	0.67
1:G:329:GLY:O	1:G:330:VAL:HG12	1.93	0.67
1:H:310:LYS:HD2	1:H:686:GLU:HB2	1.77	0.67
1:I:310:LYS:HD2	1:I:686:GLU:HB2	1.77	0.67
1:I:286:ASN:HD21	1:I:619:TRP:H	1.42	0.67
1:H:429:GLN:HE21	1:H:736:LEU:H	1.41	0.67
1:D:310:LYS:HD2	1:D:686:GLU:HB2	1.77	0.67
1:D:451:ASN:HD21	1:D:458:ASN:HB2	1.59	0.67
1:B:310:LYS:HD2	1:B:686:GLU:HB2	1.77	0.67
1:G:310:LYS:HD2	1:G:686:GLU:HB2	1.77	0.67
1:H:696:ASN:ND2	1:H:696:ASN:H	1.93	0.67
1:D:380:THR:HG22	1:H:428:SER:O	1.93	0.67
1:E:310:LYS:HD2	1:E:686:GLU:HB2	1.77	0.67
1:E:451:ASN:HD21	1:E:458:ASN:HB2	1.59	0.67
1:A:330:VAL:CG1	1:B:327:ASN:OD1	2.40	0.67
1:B:698:GLU:H	1:J:298:GLN:HE22	1.41	0.67
1:C:278:THR:CG2	1:C:280:TRP:H	2.07	0.66
1:E:218:ALA:O	1:E:219:ASP:CB	2.43	0.66
1:E:696:ASN:ND2	1:E:696:ASN:H	1.93	0.66
1:G:564:GLU:O	1:G:567:LYS:HG2	1.94	0.66
1:J:278:THR:CG2	1:J:280:TRP:H	2.07	0.66
1:A:698:GLU:H	1:E:298:GLN:HE22	1.41	0.66
1:A:310:LYS:HD2	1:A:686:GLU:HB2	1.77	0.66
1:F:502:THR:O	1:F:506:ALA:CB	2.40	0.66
1:H:286:ASN:HD21	1:H:619:TRP:H	1.42	0.66
1:J:286:ASN:HD21	1:J:619:TRP:H	1.42	0.66
1:F:310:LYS:HD2	1:F:686:GLU:HB2	1.77	0.66
1:H:278:THR:CG2	1:H:280:TRP:H	2.07	0.66
1:J:696:ASN:H	1:J:696:ASN:ND2	1.93	0.66
1:A:286:ASN:HD21	1:A:619:TRP:H	1.42	0.66
1:J:327:ASN:O	1:J:328:ASP:CB	2.40	0.66
1:B:451:ASN:HD21	1:B:458:ASN:HB2	1.59	0.66
1:C:429:GLN:HE21	1:C:736:LEU:H	1.41	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:GLY:O	1:F:218:ALA:CB	2.44	0.66
1:G:696:ASN:ND2	1:G:696:ASN:H	1.93	0.66
1:J:502:THR:O	1:J:506:ALA:CB	2.40	0.66
1:B:696:ASN:ND2	1:B:696:ASN:H	1.93	0.66
1:H:502:THR:O	1:H:506:ALA:CB	2.40	0.66
1:A:330:VAL:HG11	1:B:327:ASN:CG	2.21	0.65
1:F:696:ASN:ND2	1:F:696:ASN:H	1.93	0.65
1:A:696:ASN:ND2	1:A:696:ASN:H	1.93	0.65
1:B:628:HIS:O	3:B:739:CYT:N1	2.29	0.65
1:D:696:ASN:ND2	1:D:696:ASN:H	1.93	0.65
1:I:278:THR:CG2	1:I:280:TRP:H	2.07	0.65
1:B:354:VAL:H	1:B:646:GLN:NE2	1.95	0.65
1:F:354:VAL:H	1:F:646:GLN:NE2	1.95	0.65
1:G:354:VAL:H	1:G:646:GLN:NE2	1.95	0.65
1:I:696:ASN:ND2	1:I:696:ASN:H	1.93	0.65
1:H:304:ASN:HD21	1:H:689:LYS:HZ1	1.44	0.65
1:A:354:VAL:H	1:A:646:GLN:NE2	1.95	0.65
1:C:502:THR:O	1:C:506:ALA:CB	2.40	0.65
1:G:663:SER:OG	1:G:665:THR:HG23	1.97	0.65
1:I:304:ASN:HD21	1:I:689:LYS:HZ1	1.44	0.65
1:A:278:THR:CG2	1:A:280:TRP:H	2.07	0.65
1:A:608:GLN:HE22	1:H:625:THR:HA	1.62	0.65
3:A:738:CYT:N1	1:H:628:HIS:O	2.30	0.65
1:E:354:VAL:H	1:E:646:GLN:NE2	1.95	0.65
1:A:502:THR:O	1:A:506:ALA:CB	2.40	0.65
1:C:310:LYS:HD2	1:C:686:GLU:HB2	1.77	0.65
1:F:255:HIS:ND1	4:F:795:HOH:O	2.25	0.65
1:I:354:VAL:H	1:I:646:GLN:NE2	1.95	0.65
1:B:625:THR:HA	1:E:608:GLN:HE22	1.62	0.65
1:J:354:VAL:H	1:J:646:GLN:NE2	1.95	0.65
1:C:264:SER:OG	1:C:265:THR:N	2.30	0.65
1:G:218:ALA:HB1	1:G:219:ASP:CG	2.22	0.65
1:G:502:THR:O	1:G:506:ALA:CB	2.40	0.65
1:G:563:GLU:OE2	1:G:611:ASP:N	2.27	0.65
1:I:457:GLN:OE1	1:I:457:GLN:N	2.30	0.65
1:A:454:GLY:O	1:A:456:ALA:N	2.30	0.65
1:F:286:ASN:HD21	1:F:619:TRP:H	1.42	0.65
1:F:302:ASN:HD21	1:F:701:TYR:H	1.45	0.65
1:H:354:VAL:H	1:H:646:GLN:NE2	1.95	0.64
1:A:628:HIS:O	3:D:738:CYT:N1	2.30	0.64
1:C:328:ASP:CB	1:C:329:GLY:O	2.42	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:GLU:N	1:C:397:GLU:OE1	2.30	0.64
1:C:625:THR:HA	1:F:608:GLN:HE22	1.62	0.64
1:D:218:ALA:O	1:D:219:ASP:HB2	1.96	0.64
1:D:354:VAL:H	1:D:646:GLN:NE2	1.95	0.64
1:D:452:GLN:O	1:D:453:SER:C	2.41	0.64
1:D:625:THR:HA	1:H:608:GLN:HE22	1.61	0.64
1:D:628:HIS:O	3:H:738:CYT:N1	2.30	0.64
1:I:502:THR:O	1:I:506:ALA:CB	2.40	0.64
1:C:696:ASN:ND2	1:C:696:ASN:H	1.93	0.64
1:E:663:SER:HG	1:E:665:THR:HG23	1.62	0.64
1:G:304:ASN:HD21	1:G:689:LYS:HZ1	1.46	0.64
1:D:304:ASN:HD21	1:D:689:LYS:HZ1	1.46	0.64
1:D:397:GLU:N	1:D:397:GLU:OE1	2.30	0.64
1:D:719:GLY:O	1:F:666:LYS:NZ	2.31	0.64
1:B:502:THR:O	1:B:506:ALA:CB	2.40	0.64
1:C:628:HIS:O	3:F:738:CYT:N1	2.30	0.64
1:H:327:ASN:O	1:H:328:ASP:CB	2.46	0.64
1:I:452:GLN:O	1:I:453:SER:C	2.40	0.64
1:I:563:GLU:OE2	1:I:611:ASP:N	2.27	0.64
1:E:278:THR:CG2	1:E:280:TRP:H	2.07	0.64
1:E:625:THR:HA	1:G:608:GLN:HE22	1.62	0.64
1:F:278:THR:CG2	1:F:280:TRP:H	2.07	0.64
1:F:628:HIS:O	3:I:738:CYT:N1	2.30	0.64
1:C:327:ASN:O	1:C:328:ASP:CB	2.46	0.64
3:C:738:CYT:N1	1:I:628:HIS:O	2.31	0.64
1:F:457:GLN:OE1	1:F:457:GLN:N	2.30	0.64
1:B:452:GLN:O	1:B:453:SER:C	2.41	0.63
1:C:354:VAL:H	1:C:646:GLN:NE2	1.95	0.63
1:F:452:GLN:O	1:F:452:GLN:HG2	1.97	0.63
1:H:452:GLN:O	1:H:453:SER:C	2.41	0.63
1:C:452:GLN:O	1:C:453:SER:C	2.41	0.63
1:D:286:ASN:ND2	1:D:618:ILE:H	1.97	0.63
1:G:278:THR:CG2	1:G:280:TRP:H	2.07	0.63
1:D:502:THR:O	1:D:506:ALA:CB	2.40	0.63
1:I:286:ASN:ND2	1:I:618:ILE:H	1.97	0.63
1:F:625:THR:HA	1:I:608:GLN:HE22	1.62	0.63
1:G:286:ASN:ND2	1:G:618:ILE:H	1.97	0.63
1:E:452:GLN:O	1:E:453:SER:C	2.41	0.63
1:H:286:ASN:ND2	1:H:618:ILE:H	1.97	0.63
1:B:286:ASN:ND2	1:B:618:ILE:H	1.97	0.63
1:D:563:GLU:OE2	1:D:611:ASP:N	2.26	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:452:GLN:O	1:G:453:SER:C	2.41	0.63
1:I:327:ASN:O	1:I:330:VAL:N	2.28	0.63
1:A:286:ASN:ND2	1:A:618:ILE:H	1.97	0.63
1:A:625:THR:HA	1:D:608:GLN:HE22	1.62	0.63
1:E:286:ASN:ND2	1:E:618:ILE:H	1.97	0.63
1:E:502:THR:O	1:E:506:ALA:CB	2.40	0.63
1:I:454:GLY:O	1:I:455:SER:HB2	1.97	0.63
1:J:286:ASN:ND2	1:J:618:ILE:H	1.97	0.63
1:J:380:THR:CG2	1:J:392:SER:H	1.98	0.63
1:C:312:LEU:C	1:C:312:LEU:CD2	2.62	0.63
1:E:264:SER:O	1:E:266:GLY:N	2.32	0.63
1:B:563:GLU:OE2	1:B:611:ASP:N	2.27	0.63
1:B:608:GLN:HE22	1:G:625:THR:HA	1.62	0.63
1:A:452:GLN:O	1:A:452:GLN:HG2	1.99	0.62
1:F:312:LEU:C	1:F:312:LEU:CD2	2.62	0.62
1:F:450:GLN:CB	1:F:458:ASN:O	2.47	0.62
1:C:608:GLN:HE22	1:I:625:THR:HA	1.61	0.62
1:I:570:ASN:HD21	1:I:608:GLN:N	1.97	0.62
1:C:286:ASN:ND2	1:C:618:ILE:H	1.97	0.62
1:J:452:GLN:O	1:J:453:SER:C	2.41	0.62
1:C:570:ASN:HD21	1:C:608:GLN:N	1.97	0.62
1:G:570:ASN:HD21	1:G:608:GLN:N	1.97	0.62
1:B:278:THR:CG2	1:B:280:TRP:H	2.07	0.62
1:A:327:ASN:O	1:A:330:VAL:N	2.33	0.62
1:J:328:ASP:HB3	1:J:329:GLY:CA	2.29	0.62
1:J:570:ASN:HD21	1:J:608:GLN:N	1.97	0.62
1:B:552:ASN:ND2	1:E:447:ASN:HD22	1.98	0.62
1:C:552:ASN:ND2	1:F:447:ASN:HD22	1.98	0.62
1:D:552:ASN:ND2	1:H:447:ASN:HD22	1.98	0.62
1:H:570:ASN:HD21	1:H:608:GLN:N	1.97	0.62
1:A:328:ASP:CB	1:A:329:GLY:HA3	2.30	0.61
1:F:552:ASN:ND2	1:I:447:ASN:HD22	1.98	0.61
1:I:312:LEU:C	1:I:312:LEU:CD2	2.62	0.61
1:A:282:TYR:O	1:A:373:ILE:HG23	2.00	0.61
1:A:563:GLU:OE2	1:A:611:ASP:N	2.27	0.61
1:A:663:SER:OG	1:A:665:THR:HG23	2.00	0.61
1:B:264:SER:O	1:B:266:GLY:N	2.31	0.61
1:F:459:LYS:HZ1	1:F:587:SER:HB3	1.63	0.61
1:G:282:TYR:O	1:G:373:ILE:HG23	2.00	0.61
1:B:282:TYR:O	1:B:373:ILE:HG23	2.00	0.61
1:J:282:TYR:O	1:J:373:ILE:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ASN:HD22	1:I:552:ASN:ND2	1.98	0.61
1:D:282:TYR:O	1:D:373:ILE:HG23	2.00	0.61
1:I:282:TYR:O	1:I:373:ILE:HG23	2.00	0.61
1:E:218:ALA:C	1:E:219:ASP:OD1	2.44	0.61
1:E:304:ASN:HD21	1:E:689:LYS:HZ1	1.48	0.61
1:F:282:TYR:O	1:F:373:ILE:HG23	2.00	0.61
1:F:286:ASN:ND2	1:F:618:ILE:H	1.97	0.61
1:J:563:GLU:OE2	1:J:611:ASP:N	2.27	0.61
1:A:447:ASN:HD22	1:H:552:ASN:ND2	1.98	0.61
1:G:237:ASP:O	1:G:687:LEU:CG	2.49	0.61
1:B:448:ARG:HA	1:G:500:ASN:HD21	1.66	0.61
1:E:563:GLU:OE2	1:E:611:ASP:N	2.27	0.61
1:E:570:ASN:HD21	1:E:608:GLN:N	1.97	0.61
1:E:552:ASN:ND2	1:G:447:ASN:HD22	1.98	0.60
1:F:456:ALA:O	1:F:457:GLN:CD	2.44	0.60
1:H:563:GLU:OE2	1:H:611:ASP:N	2.26	0.60
1:I:703:SER:HB2	4:I:743:HOH:O	1.99	0.60
1:A:500:ASN:HD21	1:D:448:ARG:HA	1.66	0.60
1:A:552:ASN:ND2	1:D:447:ASN:HD22	1.98	0.60
1:B:500:ASN:HD21	1:E:448:ARG:HA	1.66	0.60
1:F:563:GLU:OE2	1:F:611:ASP:N	2.27	0.60
1:H:282:TYR:O	1:H:373:ILE:HG23	2.00	0.60
1:C:304:ASN:HD21	1:C:689:LYS:HZ1	1.47	0.60
1:D:500:ASN:HD21	1:H:448:ARG:HA	1.66	0.60
1:I:452:GLN:O	1:I:452:GLN:HG2	2.01	0.60
1:C:327:ASN:O	1:C:330:VAL:N	2.34	0.60
1:F:289:HIS:CE1	1:F:365:PRO:HG3	2.37	0.60
1:F:500:ASN:HD21	1:I:448:ARG:HA	1.66	0.60
1:G:327:ASN:O	1:G:330:VAL:N	2.34	0.60
1:G:328:ASP:CB	1:G:329:GLY:O	2.42	0.60
1:B:299:ARG:NH2	1:J:690:GLU:OE2	2.34	0.60
1:C:282:TYR:O	1:C:373:ILE:HG23	2.00	0.60
1:A:299:ARG:NH2	1:E:690:GLU:OE2	2.34	0.60
1:C:289:HIS:CE1	1:C:365:PRO:HG3	2.37	0.60
1:C:448:ARG:HA	1:I:500:ASN:HD21	1.67	0.60
1:C:500:ASN:HD21	1:F:448:ARG:HA	1.66	0.60
1:E:282:TYR:O	1:E:373:ILE:HG23	2.00	0.60
1:H:328:ASP:CB	1:H:329:GLY:O	2.42	0.60
1:E:500:ASN:HD21	1:G:448:ARG:HA	1.66	0.60
1:A:450:GLN:OE1	1:A:457:GLN:HB3	2.01	0.60
1:B:289:HIS:CE1	1:B:365:PRO:HG3	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:ASN:O	1:G:328:ASP:CB	2.46	0.60
1:A:289:HIS:CE1	1:A:365:PRO:HG3	2.37	0.60
1:A:448:ARG:HA	1:H:500:ASN:HD21	1.66	0.60
1:D:278:THR:HB	1:D:376:TYR:O	2.02	0.60
1:B:328:ASP:OD1	1:B:329:GLY:N	2.35	0.59
1:I:289:HIS:CE1	1:I:365:PRO:HG3	2.37	0.59
1:I:278:THR:HB	1:I:376:TYR:O	2.02	0.59
1:A:422:HIS:CE1	1:A:612:VAL:HG22	2.38	0.59
1:B:278:THR:HB	1:B:376:TYR:O	2.02	0.59
1:D:299:ARG:NH2	1:I:690:GLU:OE2	2.35	0.59
1:E:278:THR:HB	1:E:376:TYR:O	2.02	0.59
1:F:459:LYS:NZ	1:F:587:SER:HB3	2.16	0.59
1:G:312:LEU:C	1:G:312:LEU:CD2	2.62	0.59
1:H:289:HIS:CE1	1:H:365:PRO:HG3	2.37	0.59
1:H:422:HIS:CE1	1:H:612:VAL:HG22	2.38	0.59
1:A:278:THR:HB	1:A:376:TYR:O	2.02	0.59
1:B:447:ASN:HD22	1:G:552:ASN:ND2	1.99	0.59
1:G:397:GLU:OE2	1:G:650:LYS:NZ	2.25	0.59
1:G:422:HIS:CE1	1:G:612:VAL:HG22	2.38	0.59
1:I:405:ARG:H	1:I:408:ASN:ND2	2.00	0.59
1:J:289:HIS:CE1	1:J:365:PRO:HG3	2.37	0.59
1:C:422:HIS:CE1	1:C:612:VAL:HG22	2.38	0.59
1:E:327:ASN:O	1:E:330:VAL:HG12	2.03	0.59
1:I:397:GLU:CD	1:I:650:LYS:HE2	2.27	0.59
1:J:422:HIS:CE1	1:J:612:VAL:HG22	2.38	0.59
1:B:422:HIS:CE1	1:B:612:VAL:HG22	2.38	0.59
1:D:289:HIS:CE1	1:D:365:PRO:HG3	2.37	0.59
1:I:422:HIS:CE1	1:I:612:VAL:HG22	2.38	0.59
1:B:638:PHE:HA	2:B:737:ADE:H61	1.68	0.59
1:E:289:HIS:CE1	1:E:365:PRO:HG3	2.37	0.59
1:F:218:ALA:O	1:F:219:ASP:HB2	2.01	0.59
1:F:263:ALA:O	1:F:264:SER:HB3	2.02	0.59
1:G:289:HIS:CE1	1:G:365:PRO:HG3	2.37	0.59
1:H:327:ASN:O	1:H:330:VAL:N	2.34	0.59
1:C:278:THR:HB	1:C:376:TYR:O	2.02	0.59
1:F:570:ASN:HD21	1:F:608:GLN:N	1.97	0.59
1:B:365:PRO:HD2	4:B:756:HOH:O	2.02	0.58
1:B:690:GLU:OE2	1:J:299:ARG:NH2	2.34	0.58
1:D:570:ASN:HD21	1:D:608:GLN:N	1.97	0.58
1:A:570:ASN:HD21	1:A:608:GLN:N	1.97	0.58
1:D:690:GLU:OE2	1:I:299:ARG:NH2	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:THR:HB	1:G:376:TYR:O	2.02	0.58
1:I:402:GLN:HG2	1:I:404:LEU:CD1	2.33	0.58
1:D:422:HIS:CE1	1:D:612:VAL:HG22	2.38	0.58
1:E:719:GLY:O	1:H:666:LYS:NZ	2.35	0.58
1:H:218:ALA:O	1:H:219:ASP:HB2	2.02	0.58
1:A:690:GLU:OE2	1:E:299:ARG:NH2	2.34	0.58
1:B:570:ASN:HD21	1:B:608:GLN:N	1.97	0.58
1:F:304:ASN:ND2	1:F:687:LEU:HB3	2.18	0.58
1:H:278:THR:HB	1:H:376:TYR:O	2.02	0.58
1:F:278:THR:HB	1:F:376:TYR:O	2.02	0.58
1:F:552:ASN:HD21	1:I:447:ASN:HD22	1.52	0.58
1:J:278:THR:HB	1:J:376:TYR:O	2.02	0.58
1:E:422:HIS:CE1	1:E:612:VAL:HG22	2.38	0.58
1:F:422:HIS:CE1	1:F:612:VAL:HG22	2.38	0.58
1:J:312:LEU:C	1:J:312:LEU:CD2	2.62	0.58
1:A:217:GLY:HA3	1:A:408:ASN:CA	2.34	0.57
1:D:532:ASP:OD2	1:D:562:ASP:OD2	2.23	0.57
1:I:280:TRP:CD2	1:I:650:LYS:HD3	2.39	0.57
1:B:217:GLY:HA2	1:B:408:ASN:HA	1.86	0.57
1:J:218:ALA:CB	1:J:407:GLY:O	2.48	0.57
1:A:532:ASP:OD2	1:A:562:ASP:OD2	2.23	0.57
1:A:552:ASN:HD21	1:D:447:ASN:HD22	1.52	0.57
1:E:263:ALA:O	1:E:264:SER:HB3	2.03	0.57
1:F:452:GLN:OE1	1:F:462:LEU:HD11	2.05	0.57
1:H:381:LEU:HD12	1:H:390:ARG:HB3	1.87	0.57
1:I:254:ASN:O	1:I:255:HIS:HB2	2.04	0.57
1:A:304:ASN:HD21	1:A:689:LYS:HZ1	1.48	0.57
1:B:381:LEU:HD12	1:B:390:ARG:HB3	1.87	0.57
1:C:608:GLN:HE22	1:I:625:THR:CA	2.18	0.57
1:E:312:LEU:C	1:E:312:LEU:CD2	2.62	0.57
1:F:399:PHE:N	1:F:399:PHE:CD1	2.72	0.57
1:H:532:ASP:OD2	1:H:562:ASP:OD2	2.23	0.57
1:J:381:LEU:HD12	1:J:390:ARG:HB3	1.87	0.57
1:B:447:ASN:HD22	1:G:552:ASN:HD21	1.53	0.56
1:F:532:ASP:OD2	1:F:562:ASP:OD2	2.23	0.56
1:I:381:LEU:HD12	1:I:390:ARG:HB3	1.87	0.56
1:A:218:ALA:O	1:A:219:ASP:HB2	2.04	0.56
1:B:552:ASN:HD21	1:E:447:ASN:HD22	1.52	0.56
1:C:381:LEU:HD12	1:C:390:ARG:HB3	1.87	0.56
1:C:552:ASN:HD21	1:F:447:ASN:HD22	1.52	0.56
1:D:552:ASN:HD21	1:H:447:ASN:HD22	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:LEU:HD12	1:E:390:ARG:HB3	1.87	0.56
1:E:532:ASP:OD2	1:E:562:ASP:OD2	2.23	0.56
1:E:552:ASN:HD21	1:G:447:ASN:HD22	1.52	0.56
1:J:532:ASP:OD2	1:J:562:ASP:OD2	2.23	0.56
1:J:717:ASN:H	1:J:717:ASN:ND2	2.04	0.56
1:H:218:ALA:C	1:H:219:ASP:OD1	2.49	0.56
1:B:326:THR:HG22	1:B:327:ASN:C	2.30	0.56
1:H:296:ASP:OD1	1:H:299:ARG:NH1	2.38	0.56
1:A:264:SER:O	1:A:266:GLY:N	2.34	0.56
1:A:381:LEU:HD12	1:A:390:ARG:HB3	1.87	0.56
1:B:666:LYS:NZ	4:B:812:HOH:O	2.30	0.56
1:D:381:LEU:HD12	1:D:390:ARG:HB3	1.87	0.56
1:F:218:ALA:C	1:F:219:ASP:OD1	2.49	0.56
1:I:532:ASP:OD2	1:I:562:ASP:OD2	2.23	0.56
1:C:625:THR:CA	1:F:608:GLN:HE22	2.19	0.56
1:D:625:THR:CA	1:H:608:GLN:HE22	2.18	0.56
1:F:341:VAL:HG12	1:F:651:ASN:HD22	1.71	0.56
1:I:456:ALA:C	1:I:457:GLN:CD	2.74	0.56
1:A:447:ASN:HD22	1:H:552:ASN:HD21	1.52	0.56
1:C:532:ASP:OD2	1:C:562:ASP:OD2	2.23	0.56
1:C:563:GLU:OE2	1:C:611:ASP:N	2.27	0.56
1:E:625:THR:CA	1:G:608:GLN:HE22	2.18	0.56
1:B:625:THR:CA	1:E:608:GLN:HE22	2.18	0.55
1:F:625:THR:CA	1:I:608:GLN:HE22	2.18	0.55
1:G:717:ASN:ND2	1:G:717:ASN:H	2.04	0.55
1:A:380:THR:CG2	1:A:392:SER:H	2.09	0.55
1:B:608:GLN:HE22	1:G:625:THR:CA	2.19	0.55
1:C:447:ASN:HD22	1:I:552:ASN:HD21	1.53	0.55
1:F:295:ARG:HH11	1:F:298:GLN:HE21	1.54	0.55
1:F:381:LEU:HD12	1:F:390:ARG:HB3	1.87	0.55
1:G:381:LEU:HD12	1:G:390:ARG:HB3	1.87	0.55
1:B:532:ASP:OD2	1:B:562:ASP:OD2	2.23	0.55
1:E:302:ASN:HD21	1:E:701:TYR:H	1.54	0.55
1:E:615:GLN:H	1:E:615:GLN:HE21	1.55	0.55
1:F:512:ASN:ND2	1:I:529:ASP:H	2.03	0.55
1:I:397:GLU:OE1	1:I:650:LYS:CE	2.35	0.55
1:I:615:GLN:H	1:I:615:GLN:HE21	1.54	0.55
1:D:302:ASN:HD21	1:D:701:TYR:H	1.54	0.55
1:D:615:GLN:H	1:D:615:GLN:HE21	1.55	0.55
1:G:451:ASN:HB2	1:G:452:GLN:HB3	1.89	0.55
1:A:302:ASN:HD21	1:A:701:TYR:H	1.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:563:GLU:HG3	4:F:775:HOH:O	2.07	0.55
1:G:532:ASP:OD2	1:G:562:ASP:OD2	2.23	0.55
1:I:717:ASN:ND2	1:I:717:ASN:H	2.04	0.55
1:B:270:ASP:HA	1:B:514:ARG:HG2	1.88	0.55
1:B:529:ASP:H	1:G:512:ASN:ND2	2.03	0.55
1:B:717:ASN:ND2	1:B:717:ASN:H	2.03	0.55
1:D:265:THR:CG2	1:D:267:ALA:HB2	2.36	0.55
1:F:254:ASN:O	1:F:255:HIS:HB2	2.07	0.55
1:I:450:GLN:OE1	1:I:457:GLN:HB3	2.07	0.55
1:A:608:GLN:HE22	1:H:625:THR:CA	2.18	0.55
1:H:451:ASN:HB2	1:H:452:GLN:HB3	1.88	0.55
1:A:615:GLN:H	1:A:615:GLN:HE21	1.55	0.55
1:I:328:ASP:HA	1:I:329:GLY:O	2.05	0.55
1:E:717:ASN:ND2	1:E:717:ASN:H	2.04	0.55
1:F:615:GLN:H	1:F:615:GLN:HE21	1.55	0.55
1:A:625:THR:CA	1:D:608:GLN:HE22	2.18	0.55
1:D:327:ASN:O	1:D:328:ASP:HB2	2.07	0.55
1:E:451:ASN:HB2	1:E:452:GLN:HB3	1.89	0.55
1:H:615:GLN:H	1:H:615:GLN:HE21	1.55	0.55
1:J:451:ASN:HB2	1:J:452:GLN:HB3	1.89	0.55
1:J:663:SER:OG	1:J:665:THR:HG23	2.07	0.55
1:A:717:ASN:H	1:A:717:ASN:ND2	2.04	0.54
1:C:635:MET:H	1:F:477:ASN:HD22	1.55	0.54
1:D:717:ASN:ND2	1:D:717:ASN:H	2.03	0.54
1:E:268:SER:O	1:E:269:ASN:C	2.48	0.54
1:F:217:GLY:HA3	1:F:408:ASN:CA	2.37	0.54
1:H:563:GLU:HG3	4:H:776:HOH:O	2.07	0.54
1:B:302:ASN:HD21	1:B:701:TYR:H	1.54	0.54
1:C:717:ASN:H	1:C:717:ASN:ND2	2.04	0.54
1:D:663:SER:OG	1:D:665:THR:HG23	2.07	0.54
1:I:480:PRO:O	1:I:605:MET:HG2	2.08	0.54
1:J:296:ASP:OD1	1:J:299:ARG:NH1	2.38	0.54
1:J:480:PRO:O	1:J:605:MET:HG2	2.08	0.54
1:A:477:ASN:HD22	1:H:635:MET:H	1.56	0.54
1:C:663:SER:OG	1:C:665:THR:HG23	2.07	0.54
1:F:304:ASN:HD22	1:F:687:LEU:HB3	1.72	0.54
1:F:635:MET:H	1:I:477:ASN:HD22	1.55	0.54
1:I:302:ASN:HD21	1:I:701:TYR:H	1.54	0.54
1:A:480:PRO:O	1:A:605:MET:HG2	2.08	0.54
1:B:451:ASN:HB2	1:B:452:GLN:HB3	1.89	0.54
1:C:451:ASN:HB2	1:C:452:GLN:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:PRO:O	1:D:605:MET:HG2	2.08	0.54
1:E:218:ALA:C	1:E:219:ASP:CG	2.75	0.54
1:G:302:ASN:HD21	1:G:701:TYR:H	1.55	0.54
1:J:302:ASN:HD21	1:J:701:TYR:H	1.54	0.54
1:A:296:ASP:OD1	1:A:299:ARG:NH1	2.38	0.54
1:D:451:ASN:HB2	1:D:452:GLN:HB3	1.89	0.54
1:D:563:GLU:HG3	4:D:775:HOH:O	2.07	0.54
1:G:480:PRO:O	1:G:605:MET:HG2	2.08	0.54
1:A:451:ASN:CB	1:A:452:GLN:CB	2.78	0.54
1:A:563:GLU:HG3	4:A:773:HOH:O	2.07	0.54
1:B:477:ASN:HD22	1:G:635:MET:H	1.56	0.54
1:E:635:MET:H	1:G:477:ASN:HD22	1.56	0.54
1:G:296:ASP:OD1	1:G:299:ARG:NH1	2.38	0.54
1:C:496:ASN:ND2	1:F:585:GLN:HE22	2.03	0.54
1:C:512:ASN:ND2	1:F:529:ASP:H	2.03	0.54
1:H:480:PRO:O	1:H:605:MET:HG2	2.08	0.54
1:H:717:ASN:H	1:H:717:ASN:ND2	2.04	0.54
1:A:328:ASP:HB3	1:A:329:GLY:HA3	1.89	0.54
1:C:480:PRO:O	1:C:605:MET:HG2	2.08	0.54
1:F:717:ASN:H	1:F:717:ASN:ND2	2.04	0.54
1:I:280:TRP:NE1	1:I:650:LYS:HD3	2.22	0.54
1:E:512:ASN:ND2	1:G:529:ASP:H	2.03	0.54
1:G:615:GLN:H	1:G:615:GLN:HE21	1.55	0.54
1:I:296:ASP:OD1	1:I:299:ARG:NH1	2.38	0.54
1:I:452:GLN:O	1:I:454:GLY:CA	2.53	0.54
1:B:512:ASN:ND2	1:E:529:ASP:H	2.03	0.54
1:F:480:PRO:O	1:F:605:MET:HG2	2.08	0.54
1:G:666:LYS:NZ	1:J:719:GLY:O	2.41	0.54
1:B:615:GLN:H	1:B:615:GLN:HE21	1.55	0.53
1:B:635:MET:H	1:E:477:ASN:HD22	1.55	0.53
1:C:380:THR:CG2	1:C:392:SER:H	2.09	0.53
1:C:563:GLU:HG3	4:C:773:HOH:O	2.07	0.53
1:C:615:GLN:HE21	1:C:615:GLN:H	1.55	0.53
1:C:477:ASN:HD22	1:I:635:MET:H	1.56	0.53
1:F:353:TYR:CE2	1:F:355:LEU:HB2	2.44	0.53
1:G:353:TYR:CE2	1:G:355:LEU:HB2	2.44	0.53
1:I:570:ASN:ND2	1:I:608:GLN:H	2.02	0.53
1:J:353:TYR:CE2	1:J:355:LEU:HB2	2.44	0.53
1:B:563:GLU:HG3	4:B:773:HOH:O	2.07	0.53
1:B:639:GLY:O	2:B:737:ADE:C2	2.61	0.53
1:C:302:ASN:HD21	1:C:701:TYR:H	1.54	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:TYR:CE2	1:E:355:LEU:HB2	2.44	0.53
1:A:353:TYR:CE2	1:A:355:LEU:HB2	2.44	0.53
1:C:353:TYR:CE2	1:C:355:LEU:HB2	2.44	0.53
1:C:585:GLN:HE22	1:I:496:ASN:ND2	2.02	0.53
1:F:380:THR:CG2	1:F:392:SER:H	2.09	0.53
1:H:302:ASN:HD21	1:H:701:TYR:H	1.54	0.53
1:B:626:ASP:H	1:E:608:GLN:NE2	2.07	0.53
1:F:270:ASP:HA	1:F:514:ARG:HG2	1.91	0.53
1:A:433:ARG:NH1	1:H:272:HIS:O	2.42	0.53
1:C:280:TRP:CE2	1:C:650:LYS:HD3	2.44	0.53
1:A:280:TRP:CE2	1:A:650:LYS:HD3	2.44	0.53
1:A:500:ASN:ND2	1:D:449:THR:H	2.07	0.53
1:D:280:TRP:CE2	1:D:650:LYS:HD3	2.44	0.53
1:H:353:TYR:CE2	1:H:355:LEU:HB2	2.44	0.53
1:J:264:SER:O	1:J:266:GLY:N	2.37	0.53
1:A:635:MET:H	1:D:477:ASN:HD22	1.55	0.53
1:B:380:THR:CG2	1:B:392:SER:H	2.09	0.53
1:B:480:PRO:O	1:B:605:MET:HG2	2.08	0.53
1:I:264:SER:O	1:I:266:GLY:N	2.37	0.53
1:J:270:ASP:HA	1:J:514:ARG:HG2	1.91	0.53
1:J:615:GLN:HE21	1:J:615:GLN:H	1.55	0.53
1:A:457:GLN:NE2	1:A:457:GLN:H	2.01	0.52
1:A:626:ASP:H	1:D:608:GLN:NE2	2.07	0.52
1:B:353:TYR:CE2	1:B:355:LEU:HB2	2.44	0.52
1:C:270:ASP:HA	1:C:514:ARG:HG2	1.91	0.52
1:D:272:HIS:O	1:H:433:ARG:NH1	2.43	0.52
1:A:270:ASP:HA	1:A:514:ARG:HG2	1.91	0.52
1:B:433:ARG:NH1	1:G:272:HIS:O	2.42	0.52
1:C:608:GLN:NE2	1:I:626:ASP:H	2.07	0.52
1:D:296:ASP:OD1	1:D:299:ARG:NH1	2.38	0.52
1:D:353:TYR:CE2	1:D:355:LEU:HB2	2.44	0.52
1:F:272:HIS:O	1:I:433:ARG:NH1	2.43	0.52
1:H:280:TRP:CE2	1:H:650:LYS:HD3	2.44	0.52
1:C:500:ASN:ND2	1:F:449:THR:H	2.07	0.52
1:D:512:ASN:ND2	1:H:529:ASP:H	2.02	0.52
1:C:626:ASP:H	1:F:608:GLN:NE2	2.07	0.52
1:D:496:ASN:ND2	1:H:585:GLN:HE22	2.02	0.52
1:F:496:ASN:ND2	1:I:585:GLN:HE22	2.03	0.52
1:F:626:ASP:H	1:I:608:GLN:NE2	2.07	0.52
1:G:342:GLN:C	1:G:343:VAL:HG23	2.35	0.52
1:I:270:ASP:HA	1:I:514:ARG:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:280:TRP:CE2	1:J:650:LYS:HD3	2.44	0.52
1:E:280:TRP:CE2	1:E:650:LYS:HD3	2.44	0.52
1:F:500:ASN:ND2	1:I:449:THR:H	2.07	0.52
1:G:612:VAL:HA	4:G:842:HOH:O	2.10	0.52
1:I:402:GLN:HG2	1:I:404:LEU:HD12	1.91	0.52
1:D:270:ASP:HA	1:D:514:ARG:HG2	1.91	0.52
1:E:626:ASP:H	1:G:608:GLN:NE2	2.07	0.52
4:E:843:HOH:O	1:G:735:PRO:HD3	2.10	0.52
1:J:383:ASN:C	1:J:383:ASN:ND2	2.68	0.52
1:B:280:TRP:CE2	1:B:650:LYS:HD3	2.44	0.52
1:B:449:THR:H	1:G:500:ASN:ND2	2.07	0.52
1:B:608:GLN:NE2	1:G:626:ASP:H	2.07	0.52
1:C:433:ARG:NH2	4:C:869:HOH:O	2.43	0.52
1:A:272:HIS:O	1:D:433:ARG:NH1	2.43	0.52
1:D:635:MET:H	1:H:477:ASN:HD22	1.55	0.52
1:E:342:GLN:C	1:E:343:VAL:HG23	2.35	0.52
1:F:280:TRP:CE2	1:F:650:LYS:HD3	2.44	0.52
1:I:353:TYR:CE2	1:I:355:LEU:HB2	2.44	0.52
1:A:449:THR:H	1:H:500:ASN:ND2	2.07	0.52
1:B:500:ASN:ND2	1:E:449:THR:H	2.07	0.52
1:B:552:ASN:HD21	1:E:447:ASN:ND2	2.08	0.52
1:E:270:ASP:HA	1:E:514:ARG:HG2	1.91	0.52
1:E:272:HIS:O	1:G:433:ARG:NH1	2.42	0.52
1:J:217:GLY:HA3	1:J:408:ASN:HA	1.92	0.52
1:C:433:ARG:NH1	1:I:272:HIS:O	2.43	0.52
1:C:449:THR:H	1:I:500:ASN:ND2	2.08	0.52
1:A:249:LEU:HB2	1:A:373:ILE:HD12	1.93	0.51
1:A:447:ASN:ND2	1:H:552:ASN:HD21	2.08	0.51
1:A:570:ASN:ND2	1:A:608:GLN:H	2.02	0.51
1:H:342:GLN:C	1:H:343:VAL:HG23	2.35	0.51
1:A:552:ASN:HD21	1:D:447:ASN:ND2	2.08	0.51
1:D:626:ASP:H	1:H:608:GLN:NE2	2.07	0.51
1:G:270:ASP:HA	1:G:514:ARG:HG2	1.91	0.51
1:H:383:ASN:C	1:H:383:ASN:ND2	2.68	0.51
1:H:433:ARG:NH2	4:H:871:HOH:O	2.43	0.51
1:B:451:ASN:CB	1:B:452:GLN:HB3	2.41	0.51
1:E:500:ASN:ND2	1:G:449:THR:H	2.07	0.51
1:F:264:SER:O	1:F:265:THR:HB	2.11	0.51
1:G:280:TRP:CG	1:G:396:LEU:HD22	2.45	0.51
1:H:270:ASP:HA	1:H:514:ARG:HG2	1.91	0.51
1:I:433:ARG:NH2	4:I:873:HOH:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:ND2	1:A:618:ILE:HB	2.26	0.51
1:A:342:GLN:C	1:A:343:VAL:HG23	2.35	0.51
1:B:342:GLN:C	1:B:343:VAL:HG23	2.35	0.51
1:J:342:GLN:C	1:J:343:VAL:HG23	2.35	0.51
1:B:286:ASN:ND2	1:B:618:ILE:HB	2.26	0.51
1:C:286:ASN:ND2	1:C:618:ILE:HB	2.26	0.51
1:C:529:ASP:H	1:I:512:ASN:ND2	2.01	0.51
1:E:563:GLU:HG3	4:E:775:HOH:O	2.10	0.51
1:F:249:LEU:HB2	1:F:373:ILE:HD12	1.93	0.51
1:G:433:ARG:NH2	4:G:871:HOH:O	2.43	0.51
1:I:383:ASN:C	1:I:383:ASN:ND2	2.68	0.51
1:A:433:ARG:NH2	4:A:868:HOH:O	2.43	0.51
1:B:447:ASN:ND2	1:G:552:ASN:HD21	2.09	0.51
1:B:451:ASN:CB	1:B:452:GLN:CB	2.89	0.51
1:C:529:ASP:O	1:C:530:ASP:HB2	2.11	0.51
1:D:286:ASN:ND2	1:D:618:ILE:HB	2.26	0.51
1:D:451:ASN:CB	1:D:452:GLN:HB3	2.41	0.51
1:E:451:ASN:CB	1:E:452:GLN:HB3	2.41	0.51
1:B:326:THR:HG23	1:B:327:ASN:O	2.07	0.51
1:E:433:ARG:NH2	4:E:871:HOH:O	2.43	0.51
1:G:529:ASP:O	1:G:530:ASP:HB2	2.11	0.51
1:H:451:ASN:CB	1:H:452:GLN:CB	2.89	0.51
1:I:342:GLN:C	1:I:343:VAL:HG23	2.35	0.51
1:J:249:LEU:HB2	1:J:373:ILE:HD12	1.93	0.51
1:J:433:ARG:NH2	4:J:873:HOH:O	2.43	0.51
1:J:451:ASN:CB	1:J:452:GLN:HB3	2.41	0.51
1:A:608:GLN:NE2	1:H:626:ASP:H	2.08	0.51
1:F:552:ASN:HD21	1:I:447:ASN:ND2	2.08	0.51
1:G:451:ASN:CB	1:G:452:GLN:HB3	2.41	0.51
1:I:249:LEU:HB2	1:I:373:ILE:HD12	1.92	0.51
1:A:536:PRO:HG3	1:A:573:ALA:HB3	1.93	0.51
1:C:249:LEU:HB2	1:C:373:ILE:HD12	1.93	0.51
1:C:342:GLN:C	1:C:343:VAL:HG23	2.35	0.51
1:C:552:ASN:HD21	1:F:447:ASN:ND2	2.08	0.51
1:D:536:PRO:HG3	1:D:573:ALA:HB3	1.93	0.51
1:F:342:GLN:C	1:F:343:VAL:HG23	2.35	0.51
1:G:249:LEU:HB2	1:G:373:ILE:HD12	1.93	0.51
1:G:280:TRP:CD1	1:G:396:LEU:HD22	2.45	0.51
1:H:217:GLY:O	1:H:408:ASN:ND2	2.34	0.51
1:B:249:LEU:HB2	1:B:373:ILE:HD12	1.93	0.51
1:C:536:PRO:HG3	1:C:573:ALA:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:ASP:O	1:E:530:ASP:HB2	2.11	0.51
1:G:286:ASN:ND2	1:G:618:ILE:HB	2.26	0.51
1:G:619:TRP:CD1	1:G:619:TRP:C	2.89	0.51
1:I:563:GLU:OE2	1:I:611:ASP:CB	2.59	0.51
1:C:270:ASP:OD2	1:C:503:TRP:HZ2	1.94	0.50
1:C:272:HIS:O	1:F:433:ARG:NH1	2.43	0.50
1:D:342:GLN:C	1:D:343:VAL:HG23	2.35	0.50
1:D:552:ASN:HD21	1:H:447:ASN:ND2	2.08	0.50
1:E:286:ASN:ND2	1:E:618:ILE:HB	2.26	0.50
1:F:619:TRP:CD1	1:F:619:TRP:C	2.89	0.50
1:H:563:GLU:OE2	1:H:611:ASP:CB	2.59	0.50
1:J:286:ASN:ND2	1:J:618:ILE:HB	2.26	0.50
1:J:619:TRP:CD1	1:J:619:TRP:C	2.89	0.50
1:A:619:TRP:CD1	1:A:619:TRP:C	2.89	0.50
1:C:218:ALA:C	1:C:219:ASP:OD1	2.54	0.50
1:D:249:LEU:HB2	1:D:373:ILE:HD12	1.92	0.50
1:F:286:ASN:ND2	1:F:618:ILE:HB	2.26	0.50
1:G:559:MET:SD	1:G:725:ARG:HA	2.51	0.50
1:G:563:GLU:OE2	1:G:611:ASP:CB	2.59	0.50
1:I:404:LEU:HA	1:I:408:ASN:HD22	1.74	0.50
1:A:529:ASP:O	1:A:530:ASP:HB2	2.11	0.50
1:B:496:ASN:ND2	1:E:585:GLN:HE22	2.03	0.50
1:B:663:SER:HG	1:B:665:THR:CG2	2.16	0.50
1:E:619:TRP:CD1	1:E:619:TRP:C	2.89	0.50
1:H:501:PHE:O	1:H:505:GLY:N	2.31	0.50
1:H:619:TRP:CD1	1:H:619:TRP:C	2.89	0.50
1:C:619:TRP:CD1	1:C:619:TRP:C	2.89	0.50
1:E:296:ASP:OD1	1:E:299:ARG:NH1	2.38	0.50
1:F:563:GLU:OE2	1:F:611:ASP:CB	2.59	0.50
1:G:703:SER:HB2	4:G:742:HOH:O	2.11	0.50
1:J:529:ASP:O	1:J:530:ASP:HB2	2.11	0.50
1:B:585:GLN:HE22	1:G:496:ASN:ND2	2.03	0.50
1:D:500:ASN:ND2	1:H:449:THR:H	2.08	0.50
1:D:529:ASP:O	1:D:530:ASP:HB2	2.11	0.50
1:E:249:LEU:HB2	1:E:373:ILE:HD12	1.93	0.50
1:H:218:ALA:C	1:H:219:ASP:CG	2.79	0.50
1:H:451:ASN:CB	1:H:452:GLN:HB3	2.41	0.50
1:I:455:SER:HB3	1:I:456:ALA:HB2	1.92	0.50
1:B:563:GLU:OE2	1:B:611:ASP:CB	2.60	0.50
1:C:451:ASN:ND2	1:C:458:ASN:HB2	2.23	0.50
1:D:451:ASN:CB	1:D:452:GLN:CB	2.89	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:536:PRO:HG3	1:H:573:ALA:HB3	1.93	0.50
1:I:451:ASN:OD1	1:I:451:ASN:O	2.30	0.50
1:D:433:ARG:NH2	4:D:871:HOH:O	2.43	0.50
1:E:451:ASN:CB	1:E:452:GLN:CB	2.89	0.50
1:E:552:ASN:HD21	1:G:447:ASN:ND2	2.08	0.50
1:F:297:TRP:O	1:F:301:ILE:HG12	2.12	0.50
1:F:451:ASN:HA	1:F:452:GLN:HB3	1.65	0.50
1:I:529:ASP:O	1:I:530:ASP:HB2	2.11	0.50
1:B:619:TRP:CD1	1:B:619:TRP:C	2.89	0.50
1:D:619:TRP:CD1	1:D:619:TRP:C	2.89	0.50
1:E:703:SER:HB2	4:E:741:HOH:O	2.12	0.50
1:F:218:ALA:O	1:F:219:ASP:OD1	2.30	0.50
1:H:286:ASN:ND2	1:H:618:ILE:HB	2.26	0.50
1:I:280:TRP:CE2	1:I:650:LYS:CD	2.90	0.50
1:J:451:ASN:CB	1:J:452:GLN:CB	2.89	0.50
1:J:563:GLU:OE2	1:J:611:ASP:CB	2.59	0.50
1:A:496:ASN:ND2	1:D:585:GLN:HE22	2.03	0.50
1:C:447:ASN:ND2	1:I:552:ASN:HD21	2.08	0.50
1:D:563:GLU:OE2	1:D:611:ASP:CB	2.59	0.50
1:E:218:ALA:O	1:E:219:ASP:HB2	2.12	0.50
1:H:529:ASP:O	1:H:530:ASP:HB2	2.11	0.50
1:I:619:TRP:CD1	1:I:619:TRP:C	2.89	0.50
1:B:296:ASP:OD1	1:B:299:ARG:NH1	2.38	0.49
1:B:433:ARG:NH2	4:B:868:HOH:O	2.43	0.49
1:B:570:ASN:ND2	1:B:608:GLN:H	2.02	0.49
1:F:536:PRO:HG3	1:F:573:ALA:HB3	1.93	0.49
1:H:354:VAL:O	1:H:354:VAL:HG13	2.12	0.49
1:I:286:ASN:ND2	1:I:618:ILE:HB	2.26	0.49
1:C:563:GLU:OE2	1:C:611:ASP:CB	2.59	0.49
1:D:715:VAL:HG21	1:F:257:TYR:O	2.12	0.49
1:E:563:GLU:OE2	1:E:611:ASP:CB	2.60	0.49
1:J:536:PRO:HG3	1:J:573:ALA:HB3	1.94	0.49
1:A:563:GLU:OE2	1:A:611:ASP:CB	2.59	0.49
1:E:715:VAL:HG21	1:H:257:TYR:O	2.12	0.49
1:G:714:THR:HG22	1:G:715:VAL:O	2.12	0.49
1:H:249:LEU:HB2	1:H:373:ILE:HD12	1.93	0.49
1:J:580:VAL:HG23	1:J:596:VAL:CG2	2.43	0.49
1:B:529:ASP:O	1:B:530:ASP:HB2	2.11	0.49
1:B:536:PRO:HG3	1:B:573:ALA:HB3	1.93	0.49
1:J:714:THR:HG22	1:J:715:VAL:O	2.12	0.49
1:B:383:ASN:C	1:B:383:ASN:ND2	2.68	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:THR:HG22	1:B:715:VAL:O	2.13	0.49
1:D:714:THR:HG22	1:D:715:VAL:O	2.13	0.49
1:E:496:ASN:ND2	1:G:585:GLN:HE22	2.03	0.49
1:G:536:PRO:HG3	1:G:573:ALA:HB3	1.93	0.49
1:I:354:VAL:O	1:I:354:VAL:HG13	2.12	0.49
1:J:264:SER:OG	1:J:265:THR:N	2.46	0.49
1:A:451:ASN:OD1	1:A:451:ASN:O	2.30	0.49
1:C:270:ASP:OD2	1:C:503:TRP:CZ2	2.65	0.49
1:E:580:VAL:HG23	1:E:596:VAL:CG2	2.42	0.49
1:G:383:ASN:C	1:G:383:ASN:ND2	2.68	0.49
1:G:451:ASN:CB	1:G:452:GLN:CB	2.89	0.49
1:H:570:ASN:ND2	1:H:608:GLN:H	2.02	0.49
1:H:580:VAL:HG23	1:H:596:VAL:CG2	2.43	0.49
1:I:396:LEU:N	1:I:396:LEU:HD12	2.27	0.49
1:D:615:GLN:H	1:D:615:GLN:NE2	2.11	0.49
1:E:536:PRO:HG3	1:E:573:ALA:HB3	1.93	0.49
1:G:283:PHE:CZ	1:G:316:LEU:HD21	2.48	0.49
1:H:316:LEU:HB2	1:H:410:PHE:HB3	1.95	0.49
1:I:316:LEU:HB2	1:I:410:PHE:HB3	1.95	0.49
1:I:580:VAL:HG23	1:I:596:VAL:CG2	2.43	0.49
1:J:283:PHE:CZ	1:J:316:LEU:HD21	2.48	0.49
1:J:316:LEU:HB2	1:J:410:PHE:HB3	1.95	0.49
1:A:283:PHE:CZ	1:A:316:LEU:HD21	2.48	0.49
1:A:580:VAL:HG23	1:A:596:VAL:CG2	2.43	0.49
1:A:715:VAL:HG21	1:B:257:TYR:O	2.13	0.49
1:B:615:GLN:H	1:B:615:GLN:NE2	2.11	0.49
1:C:316:LEU:HB2	1:C:410:PHE:HB3	1.95	0.49
1:D:283:PHE:CZ	1:D:316:LEU:HD21	2.48	0.49
1:E:714:THR:HG22	1:E:715:VAL:O	2.12	0.49
1:G:278:THR:HG23	1:G:280:TRP:HD1	1.78	0.49
1:H:264:SER:O	1:H:266:GLY:N	2.36	0.49
1:H:283:PHE:CZ	1:H:316:LEU:HD21	2.48	0.49
1:I:714:THR:HG22	1:I:715:VAL:O	2.12	0.49
1:J:615:GLN:H	1:J:615:GLN:NE2	2.11	0.49
1:C:714:THR:HG22	1:C:715:VAL:O	2.12	0.49
1:G:316:LEU:HB2	1:G:410:PHE:HB3	1.95	0.49
1:G:580:VAL:HG23	1:G:596:VAL:CG2	2.43	0.49
1:A:354:VAL:O	1:A:354:VAL:HG13	2.12	0.49
1:D:257:TYR:OH	1:D:397:GLU:OE1	2.25	0.49
1:F:529:ASP:O	1:F:530:ASP:HB2	2.11	0.49
1:A:529:ASP:H	1:H:512:ASN:ND2	2.03	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ASP:OD1	1:C:299:ARG:NH1	2.38	0.48
1:C:383:ASN:C	1:C:383:ASN:ND2	2.68	0.48
1:D:327:ASN:O	1:D:330:VAL:N	2.43	0.48
1:F:580:VAL:HG23	1:F:596:VAL:CG2	2.43	0.48
1:B:316:LEU:HB2	1:B:410:PHE:HB3	1.95	0.48
1:B:580:VAL:HG23	1:B:596:VAL:CG2	2.43	0.48
1:E:283:PHE:CZ	1:E:316:LEU:HD21	2.48	0.48
1:H:714:THR:HG22	1:H:715:VAL:O	2.12	0.48
1:I:283:PHE:CZ	1:I:316:LEU:HD21	2.48	0.48
1:J:357:SER:HB3	1:J:359:HIS:CE1	2.49	0.48
1:A:328:ASP:CB	1:A:329:GLY:CA	2.91	0.48
1:A:714:THR:HG22	1:A:715:VAL:O	2.12	0.48
1:B:283:PHE:CZ	1:B:316:LEU:HD21	2.48	0.48
1:B:354:VAL:HG13	1:B:354:VAL:O	2.12	0.48
1:B:397:GLU:C	1:B:399:PHE:H	2.20	0.48
1:C:283:PHE:CZ	1:C:316:LEU:HD21	2.48	0.48
1:D:580:VAL:HG23	1:D:596:VAL:CG2	2.43	0.48
1:E:354:VAL:HG13	1:E:354:VAL:O	2.13	0.48
1:E:615:GLN:H	1:E:615:GLN:NE2	2.11	0.48
1:G:257:TYR:O	1:J:715:VAL:HG21	2.13	0.48
1:I:615:GLN:H	1:I:615:GLN:NE2	2.11	0.48
1:A:615:GLN:H	1:A:615:GLN:NE2	2.11	0.48
1:D:703:SER:HB2	4:D:741:HOH:O	2.13	0.48
1:F:714:THR:HG22	1:F:715:VAL:O	2.12	0.48
1:I:380:THR:CG2	1:I:392:SER:H	2.09	0.48
1:J:354:VAL:HG13	1:J:354:VAL:O	2.12	0.48
1:B:437:PRO:HG3	1:G:379:LEU:HG	1.95	0.48
1:B:639:GLY:O	2:B:737:ADE:H2	1.95	0.48
1:C:580:VAL:HG23	1:C:596:VAL:CG2	2.43	0.48
1:D:218:ALA:O	1:D:219:ASP:CB	2.61	0.48
1:F:283:PHE:CZ	1:F:316:LEU:HD21	2.48	0.48
1:F:316:LEU:HB2	1:F:410:PHE:HB3	1.95	0.48
1:F:354:VAL:O	1:F:354:VAL:HG13	2.12	0.48
1:H:230:CYS:HB2	1:H:244:THR:CG2	2.43	0.48
1:A:379:LEU:HG	1:D:437:PRO:HG3	1.96	0.48
1:A:585:GLN:HE22	1:H:496:ASN:ND2	2.03	0.48
1:C:218:ALA:O	1:C:219:ASP:OD1	2.30	0.48
1:C:379:LEU:HG	1:F:437:PRO:HG3	1.96	0.48
1:C:615:GLN:H	1:C:615:GLN:NE2	2.11	0.48
1:G:218:ALA:HB1	1:G:219:ASP:OD1	2.13	0.48
1:H:615:GLN:H	1:H:615:GLN:NE2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:666:LYS:O	1:H:666:LYS:HG2	2.12	0.48
1:I:536:PRO:HG3	1:I:573:ALA:HB3	1.93	0.48
3:J:738:CYT:N4	4:J:769:HOH:O	2.23	0.48
1:A:452:GLN:O	1:A:453:SER:C	2.55	0.48
1:D:354:VAL:HG13	1:D:354:VAL:O	2.12	0.48
1:H:397:GLU:C	1:H:399:PHE:H	2.21	0.48
1:A:399:PHE:CD1	1:A:399:PHE:N	2.82	0.48
1:C:264:SER:HG	1:C:265:THR:H	1.62	0.48
1:D:383:ASN:C	1:D:383:ASN:ND2	2.68	0.48
1:F:615:GLN:H	1:F:615:GLN:NE2	2.11	0.48
1:G:615:GLN:H	1:G:615:GLN:NE2	2.11	0.48
1:A:257:TYR:O	1:I:715:VAL:HG21	2.13	0.48
1:A:346:ASP:OD2	1:A:351:LEU:HB2	2.14	0.48
1:B:346:ASP:OD2	1:B:351:LEU:HB2	2.14	0.48
1:E:316:LEU:HB2	1:E:410:PHE:HB3	1.95	0.48
1:E:380:THR:CG2	1:E:392:SER:H	2.09	0.48
1:F:570:ASN:ND2	1:F:608:GLN:H	2.02	0.48
1:A:257:TYR:OH	1:A:397:GLU:OE1	2.28	0.47
1:D:635:MET:HB2	1:H:477:ASN:ND2	2.29	0.47
1:G:354:VAL:O	1:G:354:VAL:HG13	2.12	0.47
1:B:379:LEU:HG	1:E:437:PRO:HG3	1.96	0.47
1:C:635:MET:HB2	1:F:477:ASN:ND2	2.30	0.47
1:E:346:ASP:OD2	1:E:351:LEU:HB2	2.14	0.47
1:H:346:ASP:OD2	1:H:351:LEU:HB2	2.14	0.47
1:H:380:THR:CG2	1:H:392:SER:H	2.09	0.47
1:I:249:LEU:HD21	1:I:650:LYS:HA	1.97	0.47
1:F:379:LEU:HG	1:I:437:PRO:HG3	1.96	0.47
1:C:354:VAL:HG13	1:C:354:VAL:O	2.12	0.47
1:F:635:MET:HB2	1:I:477:ASN:ND2	2.29	0.47
1:G:232:SER:OG	1:G:296:ASP:OD2	2.27	0.47
1:G:346:ASP:OD2	1:G:351:LEU:HB2	2.14	0.47
1:A:262:SER:O	1:A:265:THR:HB	2.14	0.47
1:B:262:SER:O	1:B:265:THR:HB	2.13	0.47
1:B:635:MET:HB2	1:E:477:ASN:ND2	2.29	0.47
1:C:451:ASN:CB	1:C:452:GLN:HB3	2.45	0.47
1:D:316:LEU:HB2	1:D:410:PHE:HB3	1.95	0.47
1:E:379:LEU:HG	1:G:437:PRO:HG3	1.96	0.47
1:E:570:ASN:ND2	1:E:608:GLN:H	2.02	0.47
1:I:454:GLY:O	1:I:455:SER:OG	2.30	0.47
1:J:425:TYR:O	1:J:730:ARG:HG2	2.15	0.47
1:A:449:THR:HG21	1:H:501:PHE:CZ	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ASN:ND2	1:H:635:MET:HB2	2.29	0.47
1:B:425:TYR:O	1:B:730:ARG:HG2	2.15	0.47
1:D:264:SER:O	1:D:265:THR:HB	2.14	0.47
1:E:635:MET:HB2	1:G:477:ASN:ND2	2.30	0.47
1:F:397:GLU:OE2	1:F:650:LYS:NZ	2.32	0.47
1:I:218:ALA:HB1	1:I:219:ASP:OD1	2.13	0.47
1:A:635:MET:HB2	1:D:477:ASN:ND2	2.30	0.47
1:C:330:VAL:CG2	1:C:331:THR:N	2.78	0.47
1:C:425:TYR:O	1:C:730:ARG:HG2	2.15	0.47
1:C:477:ASN:ND2	1:I:635:MET:HB2	2.30	0.47
1:D:346:ASP:OD2	1:D:351:LEU:HB2	2.14	0.47
1:D:379:LEU:HG	1:H:437:PRO:HG3	1.96	0.47
1:F:295:ARG:HH11	1:F:298:GLN:NE2	2.13	0.47
1:G:264:SER:OG	1:G:265:THR:N	2.47	0.47
1:G:425:TYR:O	1:G:730:ARG:HG2	2.15	0.47
1:H:330:VAL:CG2	1:H:331:THR:N	2.78	0.47
1:H:397:GLU:OE2	1:H:650:LYS:NZ	2.41	0.47
1:I:346:ASP:OD2	1:I:351:LEU:HB2	2.14	0.47
1:J:346:ASP:OD2	1:J:351:LEU:HB2	2.14	0.47
1:A:316:LEU:HB2	1:A:410:PHE:HB3	1.95	0.47
1:A:425:TYR:O	1:A:730:ARG:HG2	2.15	0.47
1:F:635:MET:HB2	1:I:477:ASN:HD21	1.80	0.47
1:H:425:TYR:O	1:H:730:ARG:HG2	2.15	0.47
1:A:437:PRO:HG3	1:H:379:LEU:HG	1.96	0.47
1:F:425:TYR:O	1:F:730:ARG:HG2	2.15	0.47
1:I:425:TYR:O	1:I:730:ARG:HG2	2.15	0.47
1:A:328:ASP:OD1	1:A:329:GLY:HA2	2.09	0.46
1:E:425:TYR:O	1:E:730:ARG:HG2	2.15	0.46
1:F:217:GLY:HA3	1:F:408:ASN:CB	2.45	0.46
1:D:278:THR:HG22	1:D:280:TRP:N	2.15	0.46
1:D:425:TYR:O	1:D:730:ARG:HG2	2.15	0.46
1:G:380:THR:CG2	1:G:392:SER:H	2.09	0.46
1:B:226:GLY:HA3	1:B:317:PHE:CD2	2.51	0.46
1:C:701:TYR:CD2	1:C:701:TYR:C	2.94	0.46
1:I:229:HIS:HE1	4:I:810:HOH:O	1.97	0.46
1:C:346:ASP:OD2	1:C:351:LEU:HB2	2.14	0.46
1:D:570:ASN:ND2	1:D:608:GLN:H	2.02	0.46
1:E:459:LYS:NZ	1:E:587:SER:HB3	2.31	0.46
1:F:346:ASP:OD2	1:F:351:LEU:HB2	2.14	0.46
1:G:459:LYS:NZ	1:G:587:SER:HB3	2.31	0.46
1:A:217:GLY:O	1:A:218:ALA:CB	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:PHE:CE2	1:F:693:LYS:HG3	2.50	0.46
1:F:701:TYR:CD2	1:F:701:TYR:C	2.94	0.46
1:F:736:LEU:HD13	1:F:736:LEU:HA	1.82	0.46
1:A:278:THR:HG22	1:A:280:TRP:N	2.15	0.46
1:A:383:ASN:C	1:A:383:ASN:ND2	2.68	0.46
1:A:701:TYR:CD2	1:A:701:TYR:C	2.94	0.46
1:B:477:ASN:ND2	1:G:635:MET:HB2	2.30	0.46
1:C:451:ASN:CB	1:C:452:GLN:CB	2.93	0.46
1:H:226:GLY:HA3	1:H:317:PHE:CD2	2.51	0.46
1:I:396:LEU:C	1:I:398:TYR:H	2.21	0.46
1:J:570:ASN:ND2	1:J:608:GLN:H	2.02	0.46
1:C:262:SER:OG	1:C:272:HIS:HA	2.16	0.46
1:C:437:PRO:HG3	1:I:379:LEU:HG	1.96	0.46
1:D:264:SER:OG	1:D:265:THR:N	2.49	0.46
1:F:226:GLY:HA3	1:F:317:PHE:CD2	2.51	0.46
1:F:342:GLN:C	1:F:343:VAL:CG2	2.89	0.46
1:I:459:LYS:NZ	1:I:587:SER:HB3	2.31	0.46
1:A:250:PRO:HG3	1:A:372:MET:HE3	1.98	0.46
1:A:342:GLN:C	1:A:343:VAL:CG2	2.89	0.46
1:A:477:ASN:HD21	1:H:635:MET:HB2	1.81	0.46
1:C:226:GLY:HA3	1:C:317:PHE:CD2	2.51	0.46
1:C:459:LYS:NZ	1:C:587:SER:HB3	2.31	0.46
1:D:635:MET:HB2	1:H:477:ASN:HD21	1.80	0.46
1:D:701:TYR:C	1:D:701:TYR:CD2	2.94	0.46
1:E:365:PRO:HD2	4:E:758:HOH:O	2.16	0.46
1:E:628:HIS:O	3:E:738:CYT:N1	2.49	0.46
1:E:635:MET:HB2	1:G:477:ASN:HD21	1.81	0.46
1:H:365:PRO:HD2	4:H:759:HOH:O	2.16	0.46
1:I:328:ASP:OD1	1:I:328:ASP:O	2.34	0.46
1:I:666:LYS:O	1:I:666:LYS:HG2	2.16	0.46
1:A:635:MET:HB2	1:D:477:ASN:HD21	1.81	0.46
1:C:263:ALA:O	1:C:264:SER:HB3	2.15	0.46
1:F:359:HIS:NE2	1:I:436:ASN:N	2.55	0.46
1:I:250:PRO:HG3	1:I:372:MET:HE3	1.98	0.46
1:J:226:GLY:HA3	1:J:317:PHE:CD2	2.51	0.46
1:C:635:MET:HB2	1:F:477:ASN:HD21	1.81	0.46
1:D:459:LYS:NZ	1:D:587:SER:HB3	2.31	0.46
1:E:342:GLN:C	1:E:343:VAL:CG2	2.89	0.46
1:G:330:VAL:CG2	1:G:331:THR:N	2.78	0.46
1:G:342:GLN:C	1:G:343:VAL:CG2	2.89	0.46
1:J:250:PRO:HG3	1:J:372:MET:HE3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LYS:NZ	1:A:587:SER:HB3	2.31	0.45
1:E:701:TYR:C	1:E:701:TYR:CD2	2.94	0.45
1:G:263:ALA:O	1:G:264:SER:HB3	2.15	0.45
1:G:701:TYR:CD2	1:G:701:TYR:C	2.94	0.45
1:I:226:GLY:HA3	1:I:317:PHE:CD2	2.51	0.45
1:J:736:LEU:HD13	1:J:736:LEU:HA	1.83	0.45
1:B:262:SER:O	1:B:265:THR:OG1	2.34	0.45
1:B:635:MET:HB2	1:E:477:ASN:HD21	1.80	0.45
1:B:701:TYR:CD2	1:B:701:TYR:C	2.94	0.45
1:H:264:SER:OG	1:H:265:THR:N	2.49	0.45
1:I:254:ASN:O	1:I:255:HIS:CB	2.63	0.45
1:B:477:ASN:HD21	1:G:635:MET:HB2	1.81	0.45
1:F:250:PRO:HG3	1:F:372:MET:HE3	1.98	0.45
1:G:226:GLY:HA3	1:G:317:PHE:CD2	2.51	0.45
1:H:342:GLN:C	1:H:343:VAL:CG2	2.89	0.45
1:H:459:LYS:NZ	1:H:587:SER:HB3	2.31	0.45
1:I:365:PRO:HD2	4:I:760:HOH:O	2.16	0.45
1:I:701:TYR:C	1:I:701:TYR:CD2	2.94	0.45
1:J:398:TYR:CG	1:J:398:TYR:O	2.69	0.45
1:J:459:LYS:NZ	1:J:587:SER:HB3	2.31	0.45
1:A:226:GLY:HA3	1:A:317:PHE:CD2	2.51	0.45
1:C:342:GLN:C	1:C:343:VAL:CG2	2.89	0.45
1:D:226:GLY:HA3	1:D:317:PHE:CD2	2.51	0.45
1:D:380:THR:CG2	1:D:392:SER:H	2.09	0.45
1:E:226:GLY:HA3	1:E:317:PHE:CD2	2.51	0.45
1:E:267:ALA:HB1	1:E:271:ASN:HB2	1.98	0.45
1:G:250:PRO:HG3	1:G:372:MET:HE3	1.98	0.45
1:G:264:SER:O	1:G:265:THR:HB	2.15	0.45
1:G:543:PHE:HB2	1:G:559:MET:HE3	1.99	0.45
1:J:263:ALA:O	1:J:264:SER:HB3	2.17	0.45
1:J:701:TYR:C	1:J:701:TYR:CD2	2.94	0.45
1:B:262:SER:O	1:B:265:THR:CB	2.65	0.45
1:C:257:TYR:OH	1:C:397:GLU:OE1	2.23	0.45
1:D:250:PRO:HG3	1:D:372:MET:HE3	1.98	0.45
1:D:342:GLN:C	1:D:343:VAL:CG2	2.89	0.45
1:E:286:ASN:HD21	1:E:619:TRP:N	2.13	0.45
1:G:220:GLY:C	1:G:222:GLY:N	2.75	0.45
1:H:701:TYR:C	1:H:701:TYR:CD2	2.94	0.45
1:B:272:HIS:O	1:E:433:ARG:NH1	2.49	0.45
1:B:459:LYS:NZ	1:B:587:SER:HB3	2.31	0.45
1:C:250:PRO:HG3	1:C:372:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:570:ASN:ND2	1:G:608:GLN:H	2.02	0.45
1:H:286:ASN:HD21	1:H:619:TRP:N	2.13	0.45
1:A:512:ASN:ND2	1:D:529:ASP:H	2.03	0.45
1:C:477:ASN:HD21	1:I:635:MET:HB2	1.81	0.45
1:D:396:LEU:N	1:D:396:LEU:HD12	2.31	0.45
1:G:329:GLY:C	1:G:330:VAL:HG12	2.42	0.45
1:B:512:ASN:HD21	1:E:529:ASP:N	2.07	0.45
1:F:296:ASP:OD1	1:F:299:ARG:NH1	2.41	0.45
1:H:305:TRP:CE3	1:H:734:ARG:NH2	2.85	0.45
1:I:487:GLN:NE2	1:I:488:ARG:H	2.15	0.45
1:A:487:GLN:NE2	1:A:488:ARG:H	2.15	0.45
1:B:305:TRP:CE3	1:B:734:ARG:NH2	2.85	0.45
1:B:342:GLN:C	1:B:343:VAL:CG2	2.89	0.45
1:C:444:TYR:CE1	1:I:544:GLY:HA3	2.52	0.45
1:D:217:GLY:O	1:D:218:ALA:HB3	2.15	0.45
1:F:621:LYS:HB2	1:F:643:PRO:HG3	1.99	0.45
1:F:666:LYS:O	1:F:666:LYS:HG2	2.17	0.45
1:G:305:TRP:CE3	1:G:734:ARG:NH2	2.85	0.45
1:I:305:TRP:CE3	1:I:734:ARG:NH2	2.85	0.45
1:B:379:LEU:HD21	1:E:437:PRO:HB3	1.99	0.45
1:B:487:GLN:NE2	1:B:488:ARG:H	2.15	0.45
1:C:621:LYS:HB2	1:C:643:PRO:HG3	1.99	0.45
1:D:223:ASN:C	1:F:405:ARG:HD2	2.42	0.45
1:D:487:GLN:NE2	1:D:488:ARG:H	2.15	0.45
1:E:305:TRP:CE3	1:E:734:ARG:NH2	2.85	0.45
1:E:379:LEU:HD21	1:G:437:PRO:HB3	1.99	0.45
1:G:315:LYS:HE2	1:G:315:LYS:HB2	1.82	0.45
1:H:257:TYR:OH	1:H:397:GLU:OE1	2.28	0.45
1:A:305:TRP:CE3	1:A:734:ARG:NH2	2.85	0.44
1:B:585:GLN:HG3	1:G:487:GLN:NE2	2.32	0.44
1:C:570:ASN:ND2	1:C:608:GLN:H	2.02	0.44
1:H:278:THR:HG22	1:H:280:TRP:N	2.15	0.44
1:J:305:TRP:CE3	1:J:734:ARG:NH2	2.85	0.44
1:J:342:GLN:C	1:J:343:VAL:CG2	2.89	0.44
1:A:264:SER:OG	1:A:265:THR:N	2.49	0.44
1:B:397:GLU:OE1	1:B:397:GLU:N	2.50	0.44
1:C:379:LEU:HD21	1:F:437:PRO:HB3	1.99	0.44
1:C:487:GLN:NE2	1:C:488:ARG:H	2.15	0.44
1:D:286:ASN:HD21	1:D:619:TRP:N	2.13	0.44
1:F:305:TRP:CE3	1:F:734:ARG:NH2	2.85	0.44
1:F:544:GLY:HA3	1:I:444:TYR:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:423:SER:HB2	1:H:425:TYR:CE2	2.53	0.44
1:I:286:ASN:HD21	1:I:619:TRP:N	2.13	0.44
1:D:305:TRP:CE3	1:D:734:ARG:NH2	2.85	0.44
1:D:316:LEU:HD23	1:D:316:LEU:HA	1.83	0.44
1:E:512:ASN:HD21	1:G:529:ASP:N	2.07	0.44
1:F:379:LEU:HD21	1:I:437:PRO:HB3	1.99	0.44
1:G:500:ASN:HD22	1:G:500:ASN:HA	1.67	0.44
1:I:342:GLN:C	1:I:343:VAL:CG2	2.89	0.44
1:B:423:SER:HB2	1:B:425:TYR:CE2	2.53	0.44
1:B:437:PRO:HB3	1:G:379:LEU:HD21	1.98	0.44
1:C:305:TRP:CE3	1:C:734:ARG:NH2	2.85	0.44
1:E:255:HIS:ND1	4:E:795:HOH:O	2.34	0.44
1:E:487:GLN:NE2	1:G:585:GLN:HG3	2.33	0.44
1:H:451:ASN:ND2	1:H:458:ASN:HB2	2.30	0.44
1:I:423:SER:HB2	1:I:425:TYR:CE2	2.53	0.44
1:J:397:GLU:OE1	1:J:397:GLU:N	2.50	0.44
1:A:423:SER:HB2	1:A:425:TYR:CE2	2.53	0.44
1:B:250:PRO:HG3	1:B:372:MET:HE3	1.98	0.44
1:D:365:PRO:HD2	4:D:758:HOH:O	2.16	0.44
1:D:544:GLY:HA3	1:H:444:TYR:CE1	2.52	0.44
1:E:392:SER:OG	1:G:694:ARG:NH1	2.51	0.44
1:F:383:ASN:C	1:F:383:ASN:ND2	2.68	0.44
1:J:423:SER:HB2	1:J:425:TYR:CE2	2.53	0.44
1:A:398:TYR:OH	1:I:232:SER:HB2	2.17	0.44
1:A:437:PRO:HB3	1:H:379:LEU:HD21	1.99	0.44
1:A:585:GLN:HG3	1:H:487:GLN:NE2	2.33	0.44
1:A:714:THR:CG2	1:A:715:VAL:H	2.31	0.44
1:C:487:GLN:NE2	1:F:585:GLN:HG3	2.33	0.44
1:C:585:GLN:HG3	1:I:487:GLN:NE2	2.32	0.44
1:D:423:SER:HB2	1:D:425:TYR:CE2	2.53	0.44
1:F:423:SER:HB2	1:F:425:TYR:CE2	2.53	0.44
1:H:487:GLN:NE2	1:H:488:ARG:H	2.15	0.44
1:J:217:GLY:HA3	1:J:409:ASN:H	1.82	0.44
1:B:359:HIS:NE2	1:E:436:ASN:N	2.56	0.44
1:C:544:GLY:HA3	1:F:444:TYR:CE1	2.53	0.44
1:E:544:GLY:HA3	1:G:444:TYR:CE1	2.53	0.44
1:G:487:GLN:NE2	1:G:488:ARG:H	2.15	0.44
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.83	0.44
1:A:365:PRO:HD2	4:A:756:HOH:O	2.16	0.44
3:A:738:CYT:N4	4:A:768:HOH:O	2.31	0.44
1:B:714:THR:CG2	1:B:715:VAL:H	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:ALA:O	1:D:733:THR:HA	2.18	0.44
1:D:621:LYS:HB2	1:D:643:PRO:HG3	1.99	0.44
1:G:286:ASN:HD21	1:G:619:TRP:N	2.13	0.44
1:H:250:PRO:HG3	1:H:372:MET:HE3	1.98	0.44
1:I:295:ARG:HH11	1:I:298:GLN:HE21	1.66	0.44
1:A:379:LEU:HD21	1:D:437:PRO:HB3	1.99	0.44
1:B:295:ARG:HH11	1:B:298:GLN:HE21	1.66	0.44
1:C:423:SER:HB2	1:C:425:TYR:CE2	2.53	0.44
1:C:426:ALA:O	1:C:733:THR:HA	2.18	0.44
1:D:295:ARG:HH11	1:D:298:GLN:HE21	1.66	0.44
1:E:250:PRO:HG3	1:E:372:MET:HE3	1.98	0.44
1:E:397:GLU:OE2	1:E:650:LYS:NZ	2.41	0.44
1:F:254:ASN:O	1:F:255:HIS:CB	2.65	0.44
1:H:426:ALA:O	1:H:733:THR:HA	2.18	0.44
1:H:621:LYS:HB2	1:H:643:PRO:HG3	1.99	0.44
1:J:327:ASN:O	1:J:330:VAL:HG13	2.18	0.44
1:A:426:ALA:O	1:A:733:THR:HA	2.18	0.43
1:A:487:GLN:NE2	1:D:585:GLN:HG3	2.33	0.43
1:A:621:LYS:HB2	1:A:643:PRO:HG3	1.99	0.43
1:A:736:LEU:HD13	1:A:736:LEU:HA	1.83	0.43
1:B:392:SER:OG	1:E:694:ARG:NH1	2.51	0.43
1:B:621:LYS:HB2	1:B:643:PRO:HG3	1.99	0.43
1:C:295:ARG:HH11	1:C:298:GLN:HE21	1.66	0.43
1:E:487:GLN:NE2	1:E:488:ARG:H	2.15	0.43
1:F:286:ASN:HD21	1:F:618:ILE:H	1.66	0.43
1:F:392:SER:OG	1:I:694:ARG:NH1	2.50	0.43
1:G:423:SER:HB2	1:G:425:TYR:CE2	2.53	0.43
1:J:286:ASN:HD21	1:J:619:TRP:N	2.13	0.43
1:J:621:LYS:HB2	1:J:643:PRO:HG3	1.99	0.43
1:B:444:TYR:CE1	1:G:544:GLY:HA3	2.53	0.43
1:B:487:GLN:NE2	1:E:585:GLN:HG3	2.33	0.43
1:C:694:ARG:NH1	1:I:392:SER:OG	2.50	0.43
1:E:423:SER:HB2	1:E:425:TYR:CE2	2.53	0.43
1:F:487:GLN:NE2	1:I:585:GLN:HG3	2.33	0.43
1:H:286:ASN:HD21	1:H:618:ILE:H	1.66	0.43
1:I:621:LYS:HB2	1:I:643:PRO:HG3	1.99	0.43
1:J:426:ALA:O	1:J:733:THR:HA	2.18	0.43
1:A:392:SER:OG	1:D:694:ARG:NH1	2.51	0.43
1:A:544:GLY:HA3	1:D:444:TYR:CE1	2.53	0.43
1:A:719:GLY:O	1:B:666:LYS:NZ	2.50	0.43
1:D:392:SER:OG	1:H:694:ARG:NH1	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:ASN:ND2	1:E:458:ASN:HB2	2.30	0.43
1:E:621:LYS:HB2	1:E:643:PRO:HG3	1.99	0.43
1:F:487:GLN:NE2	1:F:488:ARG:H	2.15	0.43
1:H:397:GLU:C	1:H:399:PHE:N	2.76	0.43
1:H:663:SER:OG	1:H:665:THR:HG23	2.18	0.43
1:A:444:TYR:CE1	1:H:544:GLY:HA3	2.53	0.43
1:B:426:ALA:O	1:B:733:THR:HA	2.18	0.43
1:E:286:ASN:HD21	1:E:618:ILE:H	1.66	0.43
1:E:500:ASN:HD22	1:E:500:ASN:HA	1.67	0.43
1:J:455:SER:HA	1:J:456:ALA:HA	1.70	0.43
1:A:694:ARG:NH1	1:H:392:SER:OG	2.51	0.43
1:C:321:VAL:HG11	1:C:339:SER:HB3	2.00	0.43
1:C:329:GLY:C	1:C:330:VAL:HG12	2.42	0.43
1:C:714:THR:CG2	1:C:715:VAL:H	2.31	0.43
1:E:397:GLU:C	1:E:399:PHE:N	2.76	0.43
1:F:321:VAL:HG11	1:F:339:SER:HB3	2.00	0.43
1:H:363:LEU:CD2	1:H:371:PHE:CZ	3.02	0.43
1:I:263:ALA:O	1:I:264:SER:HB3	2.18	0.43
1:I:703:SER:CB	4:I:743:HOH:O	2.62	0.43
1:J:286:ASN:HD21	1:J:618:ILE:H	1.67	0.43
1:J:451:ASN:ND2	1:J:458:ASN:HB2	2.30	0.43
1:A:321:VAL:HG11	1:A:339:SER:HB3	2.00	0.43
1:B:278:THR:HG22	1:B:280:TRP:N	2.15	0.43
1:C:437:PRO:HB3	1:I:379:LEU:HD21	1.99	0.43
1:E:363:LEU:CD2	1:E:371:PHE:CZ	3.02	0.43
1:F:455:SER:HA	1:F:456:ALA:HA	1.66	0.43
1:J:363:LEU:CD2	1:J:371:PHE:CZ	3.02	0.43
1:J:436:ASN:C	1:J:436:ASN:OD1	2.61	0.43
1:J:487:GLN:NE2	1:J:488:ARG:H	2.15	0.43
1:A:217:GLY:HA3	1:A:408:ASN:HB3	2.01	0.43
1:B:397:GLU:C	1:B:399:PHE:N	2.76	0.43
1:B:544:GLY:HA3	1:E:444:TYR:CE1	2.52	0.43
1:C:392:SER:OG	1:F:694:ARG:NH1	2.51	0.43
3:D:738:CYT:N4	4:D:770:HOH:O	2.31	0.43
1:E:426:ALA:O	1:E:733:THR:HA	2.18	0.43
1:F:217:GLY:HA3	1:F:408:ASN:HB3	2.01	0.43
1:F:399:PHE:N	1:F:399:PHE:HD1	2.15	0.43
1:G:295:ARG:HH11	1:G:298:GLN:HE21	1.66	0.43
1:G:426:ALA:O	1:G:733:THR:HA	2.18	0.43
1:I:321:VAL:HG11	1:I:339:SER:HB3	2.00	0.43
1:J:321:VAL:HG11	1:J:339:SER:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:O	1:A:264:SER:HB3	2.19	0.43
1:D:379:LEU:HD21	1:H:437:PRO:HB3	1.99	0.43
1:D:487:GLN:NE2	1:H:585:GLN:HG3	2.33	0.43
1:B:363:LEU:CD2	1:B:371:PHE:CZ	3.02	0.43
1:F:426:ALA:O	1:F:733:THR:HA	2.18	0.43
1:G:621:LYS:HB2	1:G:643:PRO:HG3	1.99	0.43
1:I:363:LEU:CD2	1:I:371:PHE:CZ	3.02	0.43
1:A:286:ASN:HD21	1:A:618:ILE:H	1.66	0.43
1:A:363:LEU:CD2	1:A:371:PHE:CZ	3.02	0.43
1:A:436:ASN:N	1:H:359:HIS:NE2	2.56	0.43
1:B:694:ARG:NH1	1:G:392:SER:OG	2.51	0.43
1:E:315:LYS:HE2	1:E:315:LYS:HB2	1.82	0.43
1:G:397:GLU:C	1:G:399:PHE:H	2.26	0.43
1:A:397:GLU:OE2	1:A:650:LYS:NZ	2.41	0.42
1:B:321:VAL:HG11	1:B:339:SER:HB3	2.00	0.42
1:E:383:ASN:C	1:E:383:ASN:ND2	2.68	0.42
1:E:714:THR:CG2	1:E:715:VAL:H	2.31	0.42
1:H:397:GLU:OE1	1:H:397:GLU:N	2.50	0.42
1:I:426:ALA:O	1:I:733:THR:HA	2.18	0.42
1:A:217:GLY:HA3	1:A:408:ASN:CB	2.48	0.42
1:A:229:HIS:HB3	4:A:833:HOH:O	2.19	0.42
1:A:295:ARG:HH11	1:A:298:GLN:HE21	1.66	0.42
1:D:321:VAL:HG11	1:D:339:SER:HB3	2.00	0.42
1:G:363:LEU:CD2	1:G:371:PHE:CZ	3.02	0.42
1:H:321:VAL:HG11	1:H:339:SER:HB3	2.00	0.42
1:I:278:THR:HG22	1:I:280:TRP:N	2.15	0.42
1:D:363:LEU:CD2	1:D:371:PHE:CZ	3.02	0.42
1:E:229:HIS:HE1	4:E:808:HOH:O	2.02	0.42
1:F:218:ALA:C	1:F:219:ASP:CG	2.86	0.42
1:G:321:VAL:HG11	1:G:339:SER:HB3	2.00	0.42
1:H:295:ARG:HH11	1:H:298:GLN:HE21	1.66	0.42
1:J:229:HIS:HB3	4:J:837:HOH:O	2.19	0.42
1:B:229:HIS:HB3	4:B:833:HOH:O	2.19	0.42
1:E:321:VAL:HG11	1:E:339:SER:HB3	2.01	0.42
1:H:455:SER:HA	1:H:456:ALA:HA	1.69	0.42
1:J:295:ARG:HH11	1:J:298:GLN:HE21	1.66	0.42
1:A:312:LEU:HA	1:A:682:GLU:O	2.20	0.42
1:B:328:ASP:OD1	1:B:328:ASP:C	2.62	0.42
1:E:295:ARG:HH11	1:E:298:GLN:HE21	1.66	0.42
1:E:655:PRO:HB3	1:E:667:PHE:CE1	2.55	0.42
1:F:363:LEU:CD2	1:F:371:PHE:CZ	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:665:THR:O	1:G:666:LYS:C	2.62	0.42
1:H:263:ALA:O	1:H:264:SER:HB3	2.19	0.42
1:I:286:ASN:HD21	1:I:618:ILE:H	1.66	0.42
1:J:316:LEU:HA	1:J:316:LEU:HD23	1.83	0.42
1:A:725:ARG:HE	1:A:725:ARG:HB3	1.69	0.42
1:C:363:LEU:CD2	1:C:371:PHE:CZ	3.02	0.42
1:G:703:SER:CB	4:G:742:HOH:O	2.67	0.42
1:H:329:GLY:C	1:H:330:VAL:HG12	2.42	0.42
1:J:328:ASP:HB3	1:J:330:VAL:N	2.33	0.42
1:B:475:PRO:HA	1:G:519:ASN:O	2.20	0.42
1:C:312:LEU:HA	1:C:682:GLU:O	2.20	0.42
1:D:229:HIS:HB3	4:D:836:HOH:O	2.19	0.42
1:F:330:VAL:O	1:F:330:VAL:CG1	2.53	0.42
1:B:280:TRP:CE3	1:B:650:LYS:HB2	2.55	0.42
1:B:286:ASN:HD21	1:B:619:TRP:N	2.13	0.42
1:C:488:ARG:HB2	1:C:574:THR:HB	2.02	0.42
1:D:725:ARG:HE	1:D:725:ARG:HB3	1.69	0.42
1:E:280:TRP:CE3	1:E:650:LYS:HB2	2.55	0.42
1:F:280:TRP:CE3	1:F:650:LYS:HB2	2.55	0.42
1:F:519:ASN:O	1:I:475:PRO:HA	2.20	0.42
1:I:312:LEU:HA	1:I:682:GLU:O	2.20	0.42
1:I:488:ARG:HB2	1:I:574:THR:HB	2.02	0.42
1:J:312:LEU:HA	1:J:682:GLU:O	2.20	0.42
1:J:397:GLU:OE2	1:J:650:LYS:NZ	2.41	0.42
1:B:312:LEU:HA	1:B:682:GLU:O	2.20	0.42
1:C:475:PRO:HA	1:I:519:ASN:O	2.20	0.42
1:E:229:HIS:HB3	4:E:836:HOH:O	2.19	0.42
1:F:500:ASN:HD22	1:F:500:ASN:HA	1.67	0.42
1:F:714:THR:CG2	1:F:715:VAL:H	2.31	0.42
1:G:488:ARG:HB2	1:G:574:THR:HB	2.02	0.42
1:J:280:TRP:CE3	1:J:650:LYS:HB2	2.55	0.42
1:J:501:PHE:O	1:J:505:GLY:N	2.44	0.42
1:D:218:ALA:H	1:D:408:ASN:HD22	1.67	0.42
1:E:488:ARG:HB2	1:E:574:THR:HB	2.02	0.42
1:J:488:ARG:HB2	1:J:574:THR:HB	2.02	0.42
1:B:449:THR:H	1:G:500:ASN:HD22	1.68	0.41
1:D:312:LEU:HA	1:D:682:GLU:O	2.20	0.41
1:D:359:HIS:NE2	1:H:436:ASN:N	2.55	0.41
1:E:500:ASN:HD22	1:G:449:THR:H	1.68	0.41
1:J:257:TYR:OH	1:J:397:GLU:OE1	2.28	0.41
1:G:365:PRO:HD2	4:G:759:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:342:GLN:HG2	1:H:403:MET:HG2	2.03	0.41
1:A:327:ASN:ND2	1:I:330:VAL:HG21	2.35	0.41
1:A:488:ARG:HB2	1:A:574:THR:HB	2.02	0.41
1:A:519:ASN:O	1:D:475:PRO:HA	2.20	0.41
1:C:278:THR:HG22	1:C:280:TRP:N	2.15	0.41
1:D:286:ASN:HD21	1:D:618:ILE:H	1.66	0.41
1:E:519:ASN:O	1:G:475:PRO:HA	2.20	0.41
1:G:451:ASN:ND2	1:G:458:ASN:HB2	2.30	0.41
1:I:714:THR:CG2	1:I:715:VAL:H	2.31	0.41
1:J:339:SER:HA	4:J:835:HOH:O	2.19	0.41
1:B:519:ASN:O	1:E:475:PRO:HA	2.20	0.41
1:C:501:PHE:O	1:C:505:GLY:N	2.44	0.41
1:C:519:ASN:O	1:F:475:PRO:HA	2.20	0.41
1:D:500:ASN:HD22	1:H:449:THR:H	1.69	0.41
1:F:586:SER:HB2	4:F:825:HOH:O	2.21	0.41
1:H:488:ARG:HB2	1:H:574:THR:HB	2.02	0.41
1:J:278:THR:HG22	1:J:280:TRP:N	2.15	0.41
1:A:449:THR:H	1:H:500:ASN:HD22	1.68	0.41
3:C:738:CYT:N4	4:C:768:HOH:O	2.24	0.41
1:D:280:TRP:CE3	1:D:650:LYS:HB2	2.55	0.41
1:G:286:ASN:HD21	1:G:618:ILE:H	1.67	0.41
1:J:693:LYS:HD3	1:J:693:LYS:HA	1.89	0.41
1:A:397:GLU:OE1	1:A:397:GLU:N	2.50	0.41
1:D:519:ASN:O	1:H:475:PRO:HA	2.20	0.41
1:D:586:SER:HB2	4:D:825:HOH:O	2.21	0.41
1:E:455:SER:HA	1:E:456:ALA:HA	1.69	0.41
1:F:628:HIS:O	3:I:738:CYT:C6	2.74	0.41
1:G:501:PHE:O	1:G:505:GLY:N	2.44	0.41
1:H:280:TRP:CE3	1:H:650:LYS:HB2	2.55	0.41
1:A:500:ASN:HD22	1:D:449:THR:H	1.68	0.41
1:C:342:GLN:HG2	1:C:403:MET:HG2	2.03	0.41
1:C:459:LYS:HZ3	1:C:587:SER:HB3	1.85	0.41
1:E:278:THR:HG22	1:E:280:TRP:N	2.15	0.41
1:E:342:GLN:HG2	1:E:403:MET:HG2	2.03	0.41
1:E:725:ARG:HE	1:E:725:ARG:HB3	1.69	0.41
1:F:312:LEU:HA	1:F:682:GLU:O	2.20	0.41
1:G:315:LYS:HB3	1:G:680:SER:HB2	2.03	0.41
1:H:714:THR:CG2	1:H:715:VAL:H	2.31	0.41
1:I:280:TRP:CD1	1:I:650:LYS:HD3	2.55	0.41
1:I:315:LYS:HB3	1:I:680:SER:HB2	2.03	0.41
1:A:284:ASP:O	1:A:362:CYS:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ARG:HB2	1:B:574:THR:HB	2.02	0.41
1:F:393:PHE:HB3	1:I:696:ASN:ND2	2.36	0.41
1:F:451:ASN:OD1	1:F:458:ASN:HB2	2.21	0.41
1:H:312:LEU:HA	1:H:682:GLU:O	2.20	0.41
1:I:264:SER:O	1:I:265:THR:HB	2.21	0.41
1:A:232:SER:HB2	1:B:398:TYR:OH	2.21	0.41
1:A:280:TRP:CE3	1:A:650:LYS:HB2	2.55	0.41
1:A:508:LYS:HG2	1:A:517:ILE:HA	2.03	0.41
1:A:696:ASN:ND2	1:H:393:PHE:HB3	2.36	0.41
1:B:219:ASP:OD1	1:B:219:ASP:N	2.53	0.41
1:B:451:ASN:ND2	1:B:458:ASN:HB2	2.30	0.41
1:B:586:SER:HB2	4:B:823:HOH:O	2.21	0.41
1:C:280:TRP:CE3	1:C:650:LYS:HB2	2.55	0.41
1:D:284:ASP:O	1:D:362:CYS:HA	2.21	0.41
1:D:455:SER:HA	1:D:456:ALA:HA	1.69	0.41
1:D:508:LYS:HG2	1:D:517:ILE:HA	2.03	0.41
1:D:628:HIS:O	3:H:738:CYT:C6	2.74	0.41
1:D:714:THR:CG2	1:D:715:VAL:H	2.30	0.41
4:D:831:HOH:O	1:H:735:PRO:HD3	2.19	0.41
1:E:312:LEU:HA	1:E:682:GLU:O	2.20	0.41
1:F:315:LYS:HE2	1:F:315:LYS:HB2	1.82	0.41
1:F:500:ASN:HD22	1:I:449:THR:H	1.68	0.41
1:I:316:LEU:HD23	1:I:316:LEU:HA	1.83	0.41
1:I:363:LEU:HA	1:I:364:PRO:HD3	1.96	0.41
1:I:508:LYS:HG2	1:I:517:ILE:HA	2.03	0.41
1:J:342:GLN:HG2	1:J:403:MET:HG2	2.03	0.41
1:J:438:LEU:O	1:J:439:ILE:HD13	2.21	0.41
3:A:738:CYT:C6	1:H:628:HIS:O	2.73	0.41
1:E:315:LYS:HB3	1:E:680:SER:HB2	2.03	0.41
1:E:397:GLU:OE1	1:E:397:GLU:N	2.50	0.41
1:G:312:LEU:HA	1:G:682:GLU:O	2.20	0.41
1:J:508:LYS:HG2	1:J:517:ILE:HA	2.03	0.41
1:A:286:ASN:HD21	1:A:619:TRP:N	2.13	0.40
1:B:393:PHE:HB3	1:E:696:ASN:ND2	2.36	0.40
1:C:286:ASN:HD21	1:C:618:ILE:H	1.66	0.40
1:C:315:LYS:HB3	1:C:680:SER:HB2	2.03	0.40
1:D:360:GLN:OE1	1:H:440:ASP:HB2	2.21	0.40
1:E:366:PHE:HA	1:E:367:PRO:HD3	1.94	0.40
1:E:569:THR:OG1	1:E:570:ASN:ND2	2.55	0.40
1:E:664:ALA:O	1:E:665:THR:C	2.63	0.40
1:G:455:SER:HA	1:G:456:ALA:HA	1.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:736:LEU:HD13	1:G:736:LEU:HA	1.83	0.40
1:I:405:ARG:H	1:I:408:ASN:HD22	1.69	0.40
1:I:569:THR:OG1	1:I:570:ASN:ND2	2.55	0.40
1:C:328:ASP:CB	1:C:329:GLY:CA	2.76	0.40
1:D:315:LYS:HB3	1:D:680:SER:HB2	2.03	0.40
1:D:427:HIS:NE2	1:D:736:LEU:HD13	2.37	0.40
1:D:488:ARG:HB2	1:D:574:THR:HB	2.02	0.40
1:E:427:HIS:NE2	1:E:736:LEU:HD13	2.37	0.40
1:F:342:GLN:HG2	1:F:403:MET:HG2	2.03	0.40
1:G:586:SER:HB2	4:G:826:HOH:O	2.21	0.40
1:A:315:LYS:HB3	1:A:680:SER:HB2	2.03	0.40
1:B:472:SER:HB3	1:G:270:ASP:O	2.22	0.40
1:C:284:ASP:O	1:C:362:CYS:HA	2.21	0.40
1:C:449:THR:H	1:I:500:ASN:HD22	1.69	0.40
1:C:628:HIS:O	3:F:738:CYT:C6	2.74	0.40
1:F:315:LYS:HB3	1:F:680:SER:HB2	2.03	0.40
1:F:488:ARG:HB2	1:F:574:THR:HB	2.02	0.40
1:G:282:TYR:CE1	1:G:374:PRO:HB2	2.57	0.40
1:I:280:TRP:CZ2	1:I:650:LYS:HE3	2.56	0.40
1:I:427:HIS:NE2	1:I:736:LEU:HD13	2.37	0.40
1:A:628:HIS:O	3:D:738:CYT:C6	2.74	0.40
1:B:342:GLN:HA	1:B:402:GLN:O	2.22	0.40
1:C:282:TYR:CE1	1:C:374:PRO:HB2	2.57	0.40
3:C:738:CYT:C6	1:I:628:HIS:O	2.74	0.40
1:D:342:GLN:HA	1:D:402:GLN:O	2.22	0.40
1:D:451:ASN:ND2	1:D:458:ASN:HB2	2.30	0.40
1:E:450:GLN:OE1	1:E:457:GLN:HB3	2.22	0.40
1:G:342:GLN:HA	1:G:402:GLN:O	2.22	0.40
1:H:500:ASN:HD22	1:H:500:ASN:HA	1.67	0.40
1:I:328:ASP:CA	1:I:329:GLY:C	2.76	0.40
1:A:229:HIS:O	1:A:242:THR:HG22	2.22	0.40
1:B:315:LYS:HB3	1:B:680:SER:HB2	2.03	0.40
1:B:342:GLN:HG2	1:B:403:MET:HG2	2.03	0.40
1:B:397:GLU:OE2	1:B:650:LYS:NZ	2.41	0.40
1:D:342:GLN:HG2	1:D:403:MET:HG2	2.03	0.40
1:D:366:PHE:HA	1:D:367:PRO:HD3	1.94	0.40
1:D:393:PHE:HB3	1:H:696:ASN:ND2	2.36	0.40
1:D:450:GLN:OE1	1:D:457:GLN:HB3	2.22	0.40
1:F:282:TYR:CE1	1:F:374:PRO:HB2	2.57	0.40
1:F:284:ASP:O	1:F:362:CYS:HA	2.21	0.40
1:F:342:GLN:HA	1:F:402:GLN:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:427:HIS:NE2	1:F:736:LEU:HD13	2.37	0.40
1:F:508:LYS:HG2	1:F:517:ILE:HA	2.03	0.40
1:G:278:THR:CG2	1:G:280:TRP:HB2	2.52	0.40
1:G:284:ASP:O	1:G:362:CYS:HA	2.21	0.40
1:G:450:GLN:OE1	1:G:457:GLN:HB3	2.22	0.40
1:G:569:THR:OG1	1:G:570:ASN:ND2	2.55	0.40
1:H:282:TYR:CE1	1:H:374:PRO:HB2	2.57	0.40
1:H:450:GLN:OE1	1:H:457:GLN:HB3	2.22	0.40
3:H:738:CYT:N4	4:H:771:HOH:O	2.29	0.40
1:I:342:GLN:HG2	1:I:403:MET:HG2	2.03	0.40
1:I:396:LEU:C	1:I:398:TYR:N	2.80	0.40
1:J:450:GLN:OE1	1:J:457:GLN:HB3	2.22	0.40

There are no symmetry-related clashes.

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	518/736 (70%)	499 (96%)	15 (3%)	4 (1%)	16	31
1	B	518/736 (70%)	500 (96%)	17 (3%)	1 (0%)	43	63
1	C	518/736 (70%)	498 (96%)	18 (4%)	2 (0%)	30	49
1	D	518/736 (70%)	498 (96%)	16 (3%)	4 (1%)	16	31
1	E	518/736 (70%)	500 (96%)	16 (3%)	2 (0%)	30	49
1	F	518/736 (70%)	501 (97%)	14 (3%)	3 (1%)	21	38
1	G	518/736 (70%)	498 (96%)	16 (3%)	4 (1%)	16	31
1	H	518/736 (70%)	498 (96%)	17 (3%)	3 (1%)	21	38
1	I	518/736 (70%)	501 (97%)	12 (2%)	5 (1%)	12	24
1	J	518/736 (70%)	497 (96%)	18 (4%)	3 (1%)	21	38
All	All	5180/7360 (70%)	4990 (96%)	159 (3%)	31 (1%)	21	38

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ALA
1	A	219	ASP
1	C	328	ASP
1	E	219	ASP
1	F	218	ALA
1	F	219	ASP
1	G	221	VAL
1	G	328	ASP
1	H	219	ASP
1	H	328	ASP
1	I	221	VAL
1	I	455	SER
1	J	328	ASP
1	A	453	SER
1	B	453	SER
1	C	453	SER
1	D	453	SER
1	E	453	SER
1	G	453	SER
1	H	453	SER
1	I	453	SER
1	J	453	SER
1	D	219	ASP
1	J	218	ALA
1	D	218	ALA
1	F	406	THR
1	G	219	ASP
1	I	219	ASP
1	I	452	GLN
1	A	452	GLN
1	D	328	ASP

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	451/617 (73%)	413 (92%)	38 (8%)	10	22
1	B	451/617 (73%)	412 (91%)	39 (9%)	10	21
1	C	451/617 (73%)	413 (92%)	38 (8%)	10	22
1	D	451/617 (73%)	415 (92%)	36 (8%)	11	24
1	E	451/617 (73%)	414 (92%)	37 (8%)	10	23
1	F	451/617 (73%)	414 (92%)	37 (8%)	10	23
1	G	451/617 (73%)	415 (92%)	36 (8%)	11	24
1	H	451/617 (73%)	413 (92%)	38 (8%)	10	22
1	I	451/617 (73%)	415 (92%)	36 (8%)	11	24
1	J	451/617 (73%)	414 (92%)	37 (8%)	10	23
All	All	4510/6170 (73%)	4138 (92%)	372 (8%)	10	23

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	229	HIS
1	A	237	ASP
1	A	244	THR
1	A	246	THR
1	A	278	THR
1	A	312	LEU
1	A	313	ASN
1	A	315	LYS
1	A	319	ILE
1	A	339	SER
1	A	354	VAL
1	A	357	SER
1	A	380	THR
1	A	383	ASN
1	A	399	PHE
1	A	413	SER
1	A	431	LEU
1	A	433	ARG
1	A	457	GLN
1	A	467	SER
1	A	489	VAL
1	A	492	THR
1	A	528	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	563	GLU
1	A	570	ASN
1	A	575	GLU
1	A	589	THR
1	A	602	LEU
1	A	608	GLN
1	A	615	GLN
1	A	628	HIS
1	A	665	THR
1	A	696	ASN
1	A	707	LYS
1	A	717	ASN
1	A	725	ARG
1	A	736	LEU
1	B	223	ASN
1	B	229	HIS
1	B	230	CYS
1	B	237	ASP
1	B	244	THR
1	B	246	THR
1	B	278	THR
1	B	312	LEU
1	B	313	ASN
1	B	315	LYS
1	B	319	ILE
1	B	325	THR
1	B	339	SER
1	B	354	VAL
1	B	357	SER
1	B	380	THR
1	B	383	ASN
1	B	413	SER
1	B	431	LEU
1	B	433	ARG
1	B	452	GLN
1	B	467	SER
1	B	489	VAL
1	B	492	THR
1	B	528	LYS
1	B	563	GLU
1	B	570	ASN
1	B	575	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	589	THR
1	B	602	LEU
1	B	608	GLN
1	B	615	GLN
1	B	628	HIS
1	B	665	THR
1	B	666	LYS
1	B	696	ASN
1	B	707	LYS
1	B	717	ASN
1	B	736	LEU
1	C	223	ASN
1	C	229	HIS
1	C	237	ASP
1	C	244	THR
1	C	246	THR
1	C	278	THR
1	C	312	LEU
1	C	313	ASN
1	C	315	LYS
1	C	319	ILE
1	C	328	ASP
1	C	330	VAL
1	C	339	SER
1	C	354	VAL
1	C	357	SER
1	C	380	THR
1	C	383	ASN
1	C	413	SER
1	C	431	LEU
1	C	433	ARG
1	C	452	GLN
1	C	467	SER
1	C	489	VAL
1	C	492	THR
1	C	528	LYS
1	C	563	GLU
1	C	570	ASN
1	C	575	GLU
1	C	589	THR
1	C	602	LEU
1	C	608	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	615	GLN
1	C	628	HIS
1	C	665	THR
1	C	696	ASN
1	C	707	LYS
1	C	717	ASN
1	C	736	LEU
1	D	223	ASN
1	D	229	HIS
1	D	237	ASP
1	D	244	THR
1	D	246	THR
1	D	278	THR
1	D	312	LEU
1	D	313	ASN
1	D	315	LYS
1	D	319	ILE
1	D	339	SER
1	D	354	VAL
1	D	357	SER
1	D	380	THR
1	D	383	ASN
1	D	413	SER
1	D	431	LEU
1	D	433	ARG
1	D	452	GLN
1	D	467	SER
1	D	489	VAL
1	D	492	THR
1	D	528	LYS
1	D	563	GLU
1	D	570	ASN
1	D	575	GLU
1	D	589	THR
1	D	602	LEU
1	D	608	GLN
1	D	615	GLN
1	D	628	HIS
1	D	665	THR
1	D	696	ASN
1	D	707	LYS
1	D	717	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	736	LEU
1	E	223	ASN
1	E	229	HIS
1	E	235	LEU
1	E	237	ASP
1	E	244	THR
1	E	246	THR
1	E	278	THR
1	E	312	LEU
1	E	313	ASN
1	E	315	LYS
1	E	319	ILE
1	E	339	SER
1	E	354	VAL
1	E	357	SER
1	E	380	THR
1	E	383	ASN
1	E	413	SER
1	E	431	LEU
1	E	433	ARG
1	E	452	GLN
1	E	467	SER
1	E	489	VAL
1	E	492	THR
1	E	528	LYS
1	E	563	GLU
1	E	570	ASN
1	E	575	GLU
1	E	589	THR
1	E	602	LEU
1	E	608	GLN
1	E	615	GLN
1	E	628	HIS
1	E	665	THR
1	E	696	ASN
1	E	707	LYS
1	E	717	ASN
1	E	736	LEU
1	F	223	ASN
1	F	229	HIS
1	F	235	LEU
1	F	237	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	244	THR
1	F	246	THR
1	F	278	THR
1	F	312	LEU
1	F	313	ASN
1	F	315	LYS
1	F	319	ILE
1	F	339	SER
1	F	354	VAL
1	F	357	SER
1	F	380	THR
1	F	383	ASN
1	F	399	PHE
1	F	413	SER
1	F	431	LEU
1	F	433	ARG
1	F	467	SER
1	F	489	VAL
1	F	492	THR
1	F	528	LYS
1	F	563	GLU
1	F	570	ASN
1	F	575	GLU
1	F	589	THR
1	F	602	LEU
1	F	608	GLN
1	F	615	GLN
1	F	628	HIS
1	F	666	LYS
1	F	696	ASN
1	F	707	LYS
1	F	717	ASN
1	F	736	LEU
1	G	229	HIS
1	G	244	THR
1	G	246	THR
1	G	278	THR
1	G	312	LEU
1	G	313	ASN
1	G	315	LYS
1	G	319	ILE
1	G	328	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	330	VAL
1	G	339	SER
1	G	354	VAL
1	G	357	SER
1	G	380	THR
1	G	383	ASN
1	G	413	SER
1	G	431	LEU
1	G	433	ARG
1	G	452	GLN
1	G	467	SER
1	G	489	VAL
1	G	492	THR
1	G	528	LYS
1	G	563	GLU
1	G	570	ASN
1	G	575	GLU
1	G	589	THR
1	G	602	LEU
1	G	608	GLN
1	G	615	GLN
1	G	628	HIS
1	G	665	THR
1	G	696	ASN
1	G	707	LYS
1	G	717	ASN
1	G	736	LEU
1	H	223	ASN
1	H	237	ASP
1	H	244	THR
1	H	246	THR
1	H	278	THR
1	H	312	LEU
1	H	313	ASN
1	H	315	LYS
1	H	319	ILE
1	H	328	ASP
1	H	330	VAL
1	H	339	SER
1	H	354	VAL
1	H	357	SER
1	H	380	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	383	ASN
1	H	413	SER
1	H	431	LEU
1	H	433	ARG
1	H	452	GLN
1	H	467	SER
1	H	489	VAL
1	H	492	THR
1	H	528	LYS
1	H	563	GLU
1	H	570	ASN
1	H	575	GLU
1	H	589	THR
1	H	602	LEU
1	H	608	GLN
1	H	615	GLN
1	H	628	HIS
1	H	665	THR
1	H	666	LYS
1	H	696	ASN
1	H	707	LYS
1	H	717	ASN
1	H	736	LEU
1	I	223	ASN
1	I	229	HIS
1	I	237	ASP
1	I	244	THR
1	I	246	THR
1	I	278	THR
1	I	312	LEU
1	I	313	ASN
1	I	315	LYS
1	I	319	ILE
1	I	339	SER
1	I	354	VAL
1	I	357	SER
1	I	380	THR
1	I	383	ASN
1	I	413	SER
1	I	431	LEU
1	I	433	ARG
1	I	467	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	489	VAL
1	I	492	THR
1	I	528	LYS
1	I	563	GLU
1	I	570	ASN
1	I	575	GLU
1	I	589	THR
1	I	602	LEU
1	I	608	GLN
1	I	615	GLN
1	I	628	HIS
1	I	665	THR
1	I	666	LYS
1	I	696	ASN
1	I	707	LYS
1	I	717	ASN
1	I	736	LEU
1	J	223	ASN
1	J	229	HIS
1	J	237	ASP
1	J	244	THR
1	J	246	THR
1	J	278	THR
1	J	312	LEU
1	J	313	ASN
1	J	315	LYS
1	J	319	ILE
1	J	330	VAL
1	J	339	SER
1	J	354	VAL
1	J	357	SER
1	J	380	THR
1	J	383	ASN
1	J	413	SER
1	J	431	LEU
1	J	433	ARG
1	J	452	GLN
1	J	467	SER
1	J	489	VAL
1	J	492	THR
1	J	528	LYS
1	J	563	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	570	ASN
1	J	575	GLU
1	J	589	THR
1	J	602	LEU
1	J	608	GLN
1	J	615	GLN
1	J	628	HIS
1	J	665	THR
1	J	696	ASN
1	J	707	LYS
1	J	717	ASN
1	J	736	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (348) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	253	ASN
1	A	259	GLN
1	A	286	ASN
1	A	289	HIS
1	A	298	GLN
1	A	302	ASN
1	A	303	ASN
1	A	304	ASN
1	A	375	GLN
1	A	383	ASN
1	A	386	GLN
1	A	402	GLN
1	A	422	HIS
1	A	429	GLN
1	A	451	ASN
1	A	457	GLN
1	A	474	GLN
1	A	477	ASN
1	A	487	GLN
1	A	496	ASN
1	A	500	ASN
1	A	510	ASN
1	A	512	ASN
1	A	552	ASN
1	A	557	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	570	ASN
1	A	608	GLN
1	A	615	GLN
1	A	624	HIS
1	A	642	ASN
1	A	646	GLN
1	A	678	GLN
1	A	691	ASN
1	A	696	ASN
1	A	704	ASN
1	A	717	ASN
1	B	253	ASN
1	B	254	ASN
1	B	259	GLN
1	B	286	ASN
1	B	289	HIS
1	B	298	GLN
1	B	302	ASN
1	B	303	ASN
1	B	304	ASN
1	B	335	ASN
1	B	375	GLN
1	B	383	ASN
1	B	386	GLN
1	B	402	GLN
1	B	422	HIS
1	B	429	GLN
1	B	451	ASN
1	B	457	GLN
1	B	477	ASN
1	B	487	GLN
1	B	496	ASN
1	B	500	ASN
1	B	510	ASN
1	B	512	ASN
1	B	552	ASN
1	B	557	ASN
1	B	570	ASN
1	B	608	GLN
1	B	615	GLN
1	B	624	HIS
1	B	642	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	646	GLN
1	B	678	GLN
1	B	691	ASN
1	B	696	ASN
1	B	704	ASN
1	B	717	ASN
1	C	229	HIS
1	C	253	ASN
1	C	254	ASN
1	C	286	ASN
1	C	298	GLN
1	C	302	ASN
1	C	304	ASN
1	C	335	ASN
1	C	375	GLN
1	C	383	ASN
1	C	402	GLN
1	C	422	HIS
1	C	429	GLN
1	C	451	ASN
1	C	457	GLN
1	C	474	GLN
1	C	477	ASN
1	C	487	GLN
1	C	496	ASN
1	C	500	ASN
1	C	510	ASN
1	C	512	ASN
1	C	552	ASN
1	C	557	ASN
1	C	570	ASN
1	C	608	GLN
1	C	615	GLN
1	C	624	HIS
1	C	642	ASN
1	C	646	GLN
1	C	678	GLN
1	C	691	ASN
1	C	696	ASN
1	C	704	ASN
1	C	717	ASN
1	D	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	286	ASN
1	D	289	HIS
1	D	298	GLN
1	D	302	ASN
1	D	303	ASN
1	D	304	ASN
1	D	342	GLN
1	D	375	GLN
1	D	383	ASN
1	D	402	GLN
1	D	422	HIS
1	D	429	GLN
1	D	451	ASN
1	D	457	GLN
1	D	474	GLN
1	D	477	ASN
1	D	487	GLN
1	D	496	ASN
1	D	500	ASN
1	D	510	ASN
1	D	512	ASN
1	D	552	ASN
1	D	570	ASN
1	D	608	GLN
1	D	615	GLN
1	D	624	HIS
1	D	642	ASN
1	D	646	GLN
1	D	678	GLN
1	D	691	ASN
1	D	696	ASN
1	D	717	ASN
1	E	229	HIS
1	E	253	ASN
1	E	286	ASN
1	E	298	GLN
1	E	302	ASN
1	E	303	ASN
1	E	304	ASN
1	E	342	GLN
1	E	375	GLN
1	E	383	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	402	GLN
1	E	422	HIS
1	E	429	GLN
1	E	451	ASN
1	E	457	GLN
1	E	474	GLN
1	E	477	ASN
1	E	487	GLN
1	E	496	ASN
1	E	500	ASN
1	E	510	ASN
1	E	512	ASN
1	E	552	ASN
1	E	557	ASN
1	E	570	ASN
1	E	608	GLN
1	E	615	GLN
1	E	624	HIS
1	E	646	GLN
1	E	678	GLN
1	E	691	ASN
1	E	696	ASN
1	E	704	ASN
1	E	717	ASN
1	F	253	ASN
1	F	286	ASN
1	F	289	HIS
1	F	298	GLN
1	F	302	ASN
1	F	303	ASN
1	F	335	ASN
1	F	342	GLN
1	F	375	GLN
1	F	383	ASN
1	F	386	GLN
1	F	402	GLN
1	F	422	HIS
1	F	429	GLN
1	F	474	GLN
1	F	477	ASN
1	F	487	GLN
1	F	496	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	500	ASN
1	F	510	ASN
1	F	512	ASN
1	F	552	ASN
1	F	557	ASN
1	F	570	ASN
1	F	608	GLN
1	F	615	GLN
1	F	624	HIS
1	F	642	ASN
1	F	646	GLN
1	F	651	ASN
1	F	678	GLN
1	F	691	ASN
1	F	696	ASN
1	F	704	ASN
1	F	717	ASN
1	G	253	ASN
1	G	259	GLN
1	G	286	ASN
1	G	289	HIS
1	G	298	GLN
1	G	302	ASN
1	G	304	ASN
1	G	375	GLN
1	G	383	ASN
1	G	386	GLN
1	G	402	GLN
1	G	422	HIS
1	G	429	GLN
1	G	451	ASN
1	G	457	GLN
1	G	474	GLN
1	G	477	ASN
1	G	487	GLN
1	G	496	ASN
1	G	500	ASN
1	G	510	ASN
1	G	512	ASN
1	G	552	ASN
1	G	557	ASN
1	G	570	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	608	GLN
1	G	615	GLN
1	G	624	HIS
1	G	642	ASN
1	G	646	GLN
1	G	678	GLN
1	G	691	ASN
1	G	696	ASN
1	G	704	ASN
1	G	717	ASN
1	G	718	ASN
1	H	253	ASN
1	H	286	ASN
1	H	289	HIS
1	H	298	GLN
1	H	302	ASN
1	H	304	ASN
1	H	335	ASN
1	H	342	GLN
1	H	375	GLN
1	H	383	ASN
1	H	386	GLN
1	H	402	GLN
1	H	422	HIS
1	H	429	GLN
1	H	451	ASN
1	H	457	GLN
1	H	474	GLN
1	H	477	ASN
1	H	487	GLN
1	H	496	ASN
1	H	500	ASN
1	H	510	ASN
1	H	512	ASN
1	H	552	ASN
1	H	557	ASN
1	H	570	ASN
1	H	608	GLN
1	H	615	GLN
1	H	624	HIS
1	H	642	ASN
1	H	646	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	678	GLN
1	H	691	ASN
1	H	696	ASN
1	H	704	ASN
1	H	717	ASN
1	I	229	HIS
1	I	253	ASN
1	I	286	ASN
1	I	298	GLN
1	I	302	ASN
1	I	303	ASN
1	I	304	ASN
1	I	375	GLN
1	I	383	ASN
1	I	408	ASN
1	I	422	HIS
1	I	429	GLN
1	I	477	ASN
1	I	487	GLN
1	I	496	ASN
1	I	500	ASN
1	I	510	ASN
1	I	512	ASN
1	I	552	ASN
1	I	557	ASN
1	I	570	ASN
1	I	608	GLN
1	I	615	GLN
1	I	624	HIS
1	I	642	ASN
1	I	646	GLN
1	I	678	GLN
1	I	691	ASN
1	I	696	ASN
1	I	704	ASN
1	I	717	ASN
1	J	223	ASN
1	J	229	HIS
1	J	253	ASN
1	J	286	ASN
1	J	289	HIS
1	J	298	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	302	ASN
1	J	303	ASN
1	J	304	ASN
1	J	359	HIS
1	J	375	GLN
1	J	383	ASN
1	J	402	GLN
1	J	422	HIS
1	J	429	GLN
1	J	451	ASN
1	J	457	GLN
1	J	474	GLN
1	J	487	GLN
1	J	496	ASN
1	J	500	ASN
1	J	512	ASN
1	J	552	ASN
1	J	557	ASN
1	J	570	ASN
1	J	608	GLN
1	J	615	GLN
1	J	642	ASN
1	J	646	GLN
1	J	678	GLN
1	J	691	ASN
1	J	696	ASN
1	J	704	ASN
1	J	717	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

20 ligands are modelled in this entry.

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
3	CYT	B	738	-	7,8,8	2.12	3 (42%)	7,10,10	5.54	4 (57%)
2	ADE	E	737	-	11,11,11	1.03	1 (9%)	15,15,15	2.46	7 (46%)
2	ADE	F	737	-	11,11,11	1.02	1 (9%)	15,15,15	2.46	7 (46%)
3	CYT	F	738	-	7,8,8	2.13	3 (42%)	7,10,10	5.53	4 (57%)
2	ADE	I	737	-	11,11,11	1.03	1 (9%)	15,15,15	2.46	7 (46%)
2	ADE	B	737	-	11,11,11	1.05	1 (9%)	15,15,15	2.45	7 (46%)
3	CYT	B	739	-	7,8,8	2.14	3 (42%)	7,10,10	5.53	4 (57%)
2	ADE	H	737	-	11,11,11	1.01	1 (9%)	15,15,15	2.46	7 (46%)
2	ADE	D	737	-	11,11,11	1.04	1 (9%)	15,15,15	2.46	7 (46%)
3	CYT	J	738	-	7,8,8	2.11	3 (42%)	7,10,10	5.56	4 (57%)
2	ADE	A	737	-	11,11,11	1.03	1 (9%)	15,15,15	2.46	7 (46%)
2	ADE	G	737	-	11,11,11	1.03	1 (9%)	15,15,15	2.47	7 (46%)
2	ADE	C	737	-	11,11,11	1.02	1 (9%)	15,15,15	2.47	7 (46%)
2	ADE	J	737	-	11,11,11	1.03	1 (9%)	15,15,15	2.46	7 (46%)
3	CYT	A	738	-	7,8,8	2.12	3 (42%)	7,10,10	5.57	4 (57%)
3	CYT	C	738	-	7,8,8	2.12	3 (42%)	7,10,10	5.57	4 (57%)
3	CYT	E	738	-	7,8,8	2.11	3 (42%)	7,10,10	5.57	4 (57%)
3	CYT	I	738	-	7,8,8	2.12	3 (42%)	7,10,10	5.58	4 (57%)
3	CYT	H	738	-	7,8,8	2.13	3 (42%)	7,10,10	5.57	4 (57%)
3	CYT	D	738	-	7,8,8	2.12	3 (42%)	7,10,10	5.57	4 (57%)

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
3	CYT	B	738	-	-	-	0/1/1/1
2	ADE	E	737	-	-	-	0/2/2/2
2	ADE	F	737	-	-	-	0/2/2/2
3	CYT	F	738	-	-	-	0/1/1/1
2	ADE	I	737	-	-	-	0/2/2/2
2	ADE	B	737	-	-	-	0/2/2/2
3	CYT	B	739	-	-	-	0/1/1/1
2	ADE	H	737	-	-	-	0/2/2/2
2	ADE	D	737	-	-	-	0/2/2/2
3	CYT	J	738	-	-	-	0/1/1/1
2	ADE	A	737	-	-	-	0/2/2/2
2	ADE	G	737	-	-	-	0/2/2/2
2	ADE	C	737	-	-	-	0/2/2/2
2	ADE	J	737	-	-	-	0/2/2/2
3	CYT	A	738	-	-	-	0/1/1/1
3	CYT	C	738	-	-	-	0/1/1/1
3	CYT	E	738	-	-	-	0/1/1/1
3	CYT	I	738	-	-	-	0/1/1/1
3	CYT	H	738	-	-	-	0/1/1/1
3	CYT	D	738	-	-	-	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	739	CYT	C4-N3	-3.22	1.32	1.37
3	H	738	CYT	C4-N3	-3.21	1.32	1.37
3	A	738	CYT	C4-N3	-3.19	1.32	1.37
3	B	738	CYT	C4-N3	-3.19	1.32	1.37
3	J	738	CYT	C4-N3	-3.18	1.32	1.37
3	F	738	CYT	C4-N3	-3.17	1.32	1.37
3	I	738	CYT	C4-N3	-3.16	1.32	1.37
3	E	738	CYT	C4-N3	-3.16	1.32	1.37
3	D	738	CYT	C4-N3	-3.16	1.32	1.37
3	C	738	CYT	C4-N3	-3.16	1.32	1.37
3	F	738	CYT	C5-C6	-2.85	1.33	1.39
3	I	738	CYT	C5-C6	-2.85	1.33	1.39
3	D	738	CYT	C5-C6	-2.83	1.33	1.39
3	A	738	CYT	C5-C6	-2.83	1.33	1.39
3	C	738	CYT	C5-C6	-2.82	1.33	1.39
3	H	738	CYT	C5-C6	-2.82	1.33	1.39
3	E	738	CYT	C5-C6	-2.82	1.33	1.39
3	J	738	CYT	C5-C6	-2.81	1.33	1.39
3	B	739	CYT	C5-C6	-2.81	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	738	CYT	C5-C6	-2.80	1.33	1.39
3	B	739	CYT	C5-C4	2.59	1.43	1.39
3	D	738	CYT	C5-C4	2.56	1.43	1.39
3	C	738	CYT	C5-C4	2.55	1.43	1.39
3	B	738	CYT	C5-C4	2.55	1.43	1.39
3	A	738	CYT	C5-C4	2.55	1.43	1.39
3	H	738	CYT	C5-C4	2.54	1.43	1.39
3	J	738	CYT	C5-C4	2.54	1.43	1.39
3	I	738	CYT	C5-C4	2.54	1.43	1.39
3	F	738	CYT	C5-C4	2.53	1.43	1.39
3	E	738	CYT	C5-C4	2.50	1.43	1.39
2	B	737	ADE	C8-N7	2.37	1.37	1.32
2	I	737	ADE	C8-N7	2.32	1.37	1.32
2	D	737	ADE	C8-N7	2.30	1.36	1.32
2	A	737	ADE	C8-N7	2.29	1.36	1.32
2	E	737	ADE	C8-N7	2.29	1.36	1.32
2	J	737	ADE	C8-N7	2.28	1.36	1.32
2	F	737	ADE	C8-N7	2.27	1.36	1.32
2	H	737	ADE	C8-N7	2.27	1.36	1.32
2	G	737	ADE	C8-N7	2.27	1.36	1.32
2	C	737	ADE	C8-N7	2.26	1.36	1.32

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	738	CYT	C5-C4-N3	12.66	125.25	118.04
3	H	738	CYT	C5-C4-N3	12.63	125.23	118.04
3	D	738	CYT	C5-C4-N3	12.61	125.22	118.04
3	A	738	CYT	C5-C4-N3	12.61	125.22	118.04
3	E	738	CYT	C5-C4-N3	12.59	125.21	118.04
3	C	738	CYT	C5-C4-N3	12.58	125.20	118.04
3	J	738	CYT	C5-C4-N3	12.56	125.20	118.04
3	F	738	CYT	C5-C4-N3	12.52	125.17	118.04
3	B	738	CYT	C5-C4-N3	12.51	125.17	118.04
3	B	739	CYT	C5-C4-N3	12.51	125.17	118.04
3	C	738	CYT	C5-C6-N1	-5.67	120.27	124.75
3	E	738	CYT	C5-C6-N1	-5.64	120.28	124.75
3	J	738	CYT	C5-C6-N1	-5.63	120.30	124.75
3	A	738	CYT	C5-C6-N1	-5.62	120.30	124.75
3	D	738	CYT	C5-C6-N1	-5.62	120.30	124.75
3	B	738	CYT	C5-C6-N1	-5.62	120.31	124.75
3	H	738	CYT	C5-C6-N1	-5.61	120.31	124.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	739	CYT	C5-C6-N1	-5.59	120.33	124.75
3	F	738	CYT	C5-C6-N1	-5.57	120.34	124.75
3	I	738	CYT	C5-C6-N1	-5.56	120.35	124.75
2	I	737	ADE	N3-C2-N1	-4.47	121.82	128.58
2	E	737	ADE	N3-C2-N1	-4.47	121.82	128.58
2	D	737	ADE	N3-C2-N1	-4.47	121.82	128.58
2	A	737	ADE	N3-C2-N1	-4.46	121.83	128.58
2	G	737	ADE	N3-C2-N1	-4.46	121.83	128.58
2	C	737	ADE	N3-C2-N1	-4.45	121.85	128.58
2	F	737	ADE	N3-C2-N1	-4.45	121.85	128.58
2	H	737	ADE	N3-C2-N1	-4.43	121.87	128.58
2	B	737	ADE	N3-C2-N1	-4.43	121.87	128.58
2	J	737	ADE	N3-C2-N1	-4.42	121.89	128.58
2	C	737	ADE	C5-N7-C8	4.30	108.33	103.48
2	J	737	ADE	C5-N7-C8	4.27	108.30	103.48
2	F	737	ADE	C5-N7-C8	4.27	108.30	103.48
2	D	737	ADE	C5-N7-C8	4.25	108.28	103.48
2	E	737	ADE	C5-N7-C8	4.25	108.27	103.48
2	G	737	ADE	C5-N7-C8	4.24	108.27	103.48
2	A	737	ADE	C5-N7-C8	4.24	108.27	103.48
2	H	737	ADE	C5-N7-C8	4.23	108.26	103.48
2	B	737	ADE	C5-N7-C8	4.22	108.24	103.48
2	I	737	ADE	C5-N7-C8	4.21	108.23	103.48
2	G	737	ADE	C5-C4-N9	3.88	110.85	105.67
2	I	737	ADE	C5-C4-N9	3.88	110.85	105.67
2	J	737	ADE	C5-C4-N9	3.86	110.83	105.67
2	C	737	ADE	C5-C4-N9	3.86	110.83	105.67
2	B	737	ADE	C5-C4-N9	3.86	110.82	105.67
2	D	737	ADE	C5-C4-N9	3.85	110.82	105.67
2	A	737	ADE	C5-C4-N9	3.85	110.82	105.67
2	H	737	ADE	C5-C4-N9	3.85	110.81	105.67
2	E	737	ADE	C5-C4-N9	3.82	110.78	105.67
2	F	737	ADE	C5-C4-N9	3.82	110.78	105.67
2	G	737	ADE	C4-C5-N7	-3.78	105.42	110.67
2	C	737	ADE	C4-C5-N7	-3.77	105.43	110.67
2	H	737	ADE	C4-C5-N7	-3.77	105.44	110.67
2	I	737	ADE	C4-C5-N7	-3.77	105.44	110.67
2	J	737	ADE	C4-C5-N7	-3.76	105.44	110.67
2	E	737	ADE	C4-C5-N7	-3.76	105.45	110.67
2	F	737	ADE	C4-C5-N7	-3.75	105.47	110.67
2	A	737	ADE	C4-C5-N7	-3.75	105.47	110.67
2	D	737	ADE	C4-C5-N7	-3.72	105.50	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	737	ADE	C4-C5-N7	-3.71	105.52	110.67
3	J	738	CYT	C6-N1-C2	3.14	123.59	118.88
3	C	738	CYT	C6-N1-C2	3.12	123.57	118.88
3	B	738	CYT	C6-N1-C2	3.12	123.56	118.88
3	E	738	CYT	C6-N1-C2	3.11	123.55	118.88
3	B	739	CYT	C6-N1-C2	3.11	123.55	118.88
3	A	738	CYT	C6-N1-C2	3.11	123.55	118.88
3	D	738	CYT	C6-N1-C2	3.10	123.54	118.88
3	I	738	CYT	C6-N1-C2	3.09	123.52	118.88
3	H	738	CYT	C6-N1-C2	3.08	123.50	118.88
3	F	738	CYT	C6-N1-C2	3.05	123.47	118.88
2	D	737	ADE	N9-C8-N7	-2.88	109.48	113.87
2	C	737	ADE	N9-C8-N7	-2.88	109.49	113.87
2	B	737	ADE	N9-C8-N7	-2.86	109.52	113.87
2	I	737	ADE	N9-C8-N7	-2.85	109.53	113.87
2	A	737	ADE	N9-C8-N7	-2.85	109.53	113.87
2	J	737	ADE	N9-C8-N7	-2.84	109.54	113.87
2	F	737	ADE	N9-C8-N7	-2.84	109.55	113.87
2	E	737	ADE	N9-C8-N7	-2.84	109.55	113.87
2	G	737	ADE	N9-C8-N7	-2.83	109.56	113.87
2	H	737	ADE	N9-C8-N7	-2.81	109.58	113.87
3	B	738	CYT	C5-C4-N4	-2.81	121.14	123.88
3	D	738	CYT	C5-C4-N4	-2.78	121.17	123.88
3	B	739	CYT	C5-C4-N4	-2.77	121.18	123.88
3	J	738	CYT	C5-C4-N4	-2.77	121.19	123.88
3	H	738	CYT	C5-C4-N4	-2.77	121.19	123.88
3	A	738	CYT	C5-C4-N4	-2.76	121.19	123.88
3	F	738	CYT	C5-C4-N4	-2.75	121.20	123.88
3	I	738	CYT	C5-C4-N4	-2.75	121.20	123.88
3	E	738	CYT	C5-C4-N4	-2.74	121.21	123.88
3	C	738	CYT	C5-C4-N4	-2.73	121.22	123.88
2	H	737	ADE	C5-C4-N3	-2.41	122.35	126.75
2	I	737	ADE	C5-C4-N3	-2.41	122.35	126.75
2	G	737	ADE	C5-C4-N3	-2.41	122.36	126.75
2	J	737	ADE	C5-C4-N3	-2.41	122.37	126.75
2	A	737	ADE	C5-C4-N3	-2.40	122.38	126.75
2	E	737	ADE	C5-C4-N3	-2.40	122.38	126.75
2	D	737	ADE	C5-C4-N3	-2.39	122.39	126.75
2	F	737	ADE	C5-C4-N3	-2.38	122.42	126.75
2	C	737	ADE	C5-C4-N3	-2.37	122.42	126.75
2	B	737	ADE	C5-C4-N3	-2.37	122.43	126.75
2	F	737	ADE	C6-C5-N7	2.24	136.42	132.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	737	ADE	C6-C5-N7	2.24	136.41	132.09
2	J	737	ADE	C6-C5-N7	2.23	136.39	132.09
2	C	737	ADE	C6-C5-N7	2.23	136.39	132.09
2	H	737	ADE	C6-C5-N7	2.23	136.38	132.09
2	G	737	ADE	C6-C5-N7	2.22	136.38	132.09
2	A	737	ADE	C6-C5-N7	2.21	136.35	132.09
2	B	737	ADE	C6-C5-N7	2.20	136.34	132.09
2	D	737	ADE	C6-C5-N7	2.20	136.33	132.09
2	I	737	ADE	C6-C5-N7	2.19	136.32	132.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	738	CYT	2	0
2	B	737	ADE	3	0
3	B	739	CYT	1	0
3	J	738	CYT	1	0
3	A	738	CYT	3	0
3	C	738	CYT	3	0
3	E	738	CYT	1	0
3	I	738	CYT	2	0
3	H	738	CYT	3	0
3	D	738	CYT	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	520/736 (70%)	0.95	54 (10%) 11 10	25, 34, 55, 92	0
1	B	520/736 (70%)	1.52	109 (20%) 2 2	25, 34, 55, 92	0
1	C	520/736 (70%)	1.74	147 (28%) 1 1	25, 34, 55, 92	0
1	D	520/736 (70%)	1.42	86 (16%) 4 3	25, 34, 55, 92	0
1	E	520/736 (70%)	2.02	224 (43%) 0 0	25, 34, 55, 92	0
1	F	520/736 (70%)	1.57	117 (22%) 2 2	25, 34, 55, 92	0
1	G	520/736 (70%)	1.88	178 (34%) 1 1	25, 34, 55, 92	0
1	H	520/736 (70%)	1.37	88 (16%) 4 3	25, 34, 55, 92	0
1	I	520/736 (70%)	1.87	173 (33%) 1 1	25, 34, 55, 92	0
1	J	520/736 (70%)	2.36	309 (59%) 0 0	25, 34, 55, 92	0
All	All	5200/7360 (70%)	1.67	1485 (28%) 1 1	25, 34, 55, 92	0

All (1485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	GLY	10.7
1	H	453	SER	10.2
1	E	217	GLY	10.1
1	F	456	ALA	10.0
1	B	218	ALA	9.5
1	J	456	ALA	9.3
1	G	218	ALA	9.0
1	I	217	GLY	9.0
1	D	218	ALA	9.0
1	H	456	ALA	8.9
1	G	456	ALA	8.9
1	F	453	SER	8.4
1	J	217	GLY	8.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	218	ALA	8.1
1	I	456	ALA	7.9
1	B	456	ALA	7.8
1	D	217	GLY	7.8
1	E	456	ALA	7.7
1	I	218	ALA	7.4
1	J	218	ALA	7.3
1	G	220	GLY	7.3
1	C	456	ALA	7.3
1	H	217	GLY	7.3
1	E	218	ALA	7.2
1	A	330	VAL	7.2
1	F	457	GLN	7.1
1	D	456	ALA	7.0
1	H	218	ALA	6.9
1	C	454	GLY	6.9
1	B	327	ASN	6.8
1	B	454	GLY	6.5
1	C	705	TYR	6.5
1	I	455	SER	6.4
1	B	217	GLY	6.4
1	C	329	GLY	6.4
1	F	454	GLY	6.4
1	I	452	GLN	6.3
1	B	452	GLN	6.3
1	F	452	GLN	6.2
1	D	454	GLY	6.0
1	F	218	ALA	6.0
1	A	455	SER	5.9
1	G	330	VAL	5.9
1	E	454	GLY	5.9
1	B	455	SER	5.8
1	G	454	GLY	5.8
1	E	453	SER	5.8
1	E	455	SER	5.8
1	H	452	GLN	5.8
1	E	705	TYR	5.7
1	H	454	GLY	5.7
1	J	455	SER	5.7
1	G	457	GLN	5.7
1	J	452	GLN	5.7
1	J	705	TYR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	330	VAL	5.6
1	G	329	GLY	5.6
1	C	453	SER	5.6
1	F	455	SER	5.5
1	F	223	ASN	5.5
1	I	330	VAL	5.5
1	I	453	SER	5.5
1	A	329	GLY	5.5
1	F	329	GLY	5.5
1	E	452	GLN	5.5
1	H	229	HIS	5.5
1	D	327	ASN	5.5
1	G	453	SER	5.4
1	J	656	ALA	5.4
1	I	454	GLY	5.4
1	J	454	GLY	5.4
1	D	452	GLN	5.3
1	H	265	THR	5.3
1	G	704	ASN	5.3
1	C	457	GLN	5.2
1	J	706	ALA	5.2
1	I	705	TYR	5.2
1	D	332	THR	5.2
1	A	218	ALA	5.1
1	H	705	TYR	5.1
1	H	457	GLN	5.1
1	I	457	GLN	5.1
1	I	265	THR	5.1
1	J	265	THR	5.1
1	I	706	ALA	5.1
1	D	453	SER	5.0
1	J	219	ASP	5.0
1	D	265	THR	5.0
1	J	451	ASN	5.0
1	G	327	ASN	4.9
1	I	327	ASN	4.9
1	G	455	SER	4.9
1	E	327	ASN	4.9
1	G	236	GLY	4.9
1	B	532	ASP	4.9
1	D	328	ASP	4.9
1	A	452	GLN	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	454	GLY	4.9
1	D	556	ASP	4.9
1	I	502	THR	4.9
1	C	458	ASN	4.9
1	D	219	ASP	4.8
1	E	641	LYS	4.8
1	F	502	THR	4.8
1	C	455	SER	4.8
1	J	327	ASN	4.8
1	E	329	GLY	4.8
1	B	329	GLY	4.7
1	H	455	SER	4.7
1	H	328	ASP	4.7
1	C	452	GLN	4.7
1	F	327	ASN	4.7
1	E	219	ASP	4.7
1	J	556	ASP	4.7
1	I	361	GLY	4.7
1	G	452	GLN	4.6
1	A	331	THR	4.6
1	G	423	SER	4.6
1	C	229	HIS	4.6
1	G	229	HIS	4.6
1	E	330	VAL	4.5
1	J	366	PHE	4.5
1	C	499	SER	4.5
1	J	704	ASN	4.5
1	F	705	TYR	4.5
1	C	330	VAL	4.5
1	G	217	GLY	4.5
1	G	451	ASN	4.5
1	J	703	SER	4.5
1	C	328	ASP	4.5
1	C	494	THR	4.5
1	G	325	THR	4.5
1	E	326	THR	4.5
1	E	532	ASP	4.5
1	J	229	HIS	4.4
1	B	264	SER	4.4
1	J	323	GLU	4.4
1	A	328	ASP	4.4
1	B	502	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	532	ASP	4.4
1	I	328	ASP	4.4
1	B	330	VAL	4.4
1	I	546	GLU	4.4
1	E	328	ASP	4.4
1	I	532	ASP	4.4
1	A	217	GLY	4.3
1	G	705	TYR	4.3
1	C	556	ASP	4.3
1	A	325	THR	4.3
1	G	546	GLU	4.3
1	F	264	SER	4.3
1	E	539	GLY	4.3
1	J	329	GLY	4.3
1	D	451	ASN	4.3
1	E	458	ASN	4.3
1	J	662	PHE	4.3
1	G	235	LEU	4.3
1	D	455	SER	4.3
1	B	220	GLY	4.2
1	F	265	THR	4.2
1	E	264	SER	4.2
1	J	453	SER	4.2
1	B	325	THR	4.2
1	E	502	THR	4.2
1	J	331	THR	4.2
1	A	456	ALA	4.2
1	I	334	ALA	4.2
1	J	507	SER	4.2
1	I	323	GLU	4.2
1	E	656	ALA	4.2
1	I	628	HIS	4.2
1	J	660	ALA	4.1
1	B	232	SER	4.1
1	D	330	VAL	4.1
1	B	457	GLN	4.1
1	A	219	ASP	4.1
1	A	264	SER	4.1
1	G	264	SER	4.1
1	D	325	THR	4.1
1	G	331	THR	4.1
1	I	592	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	458	ASN	4.1
1	G	710	ASN	4.1
1	H	219	ASP	4.1
1	E	396	LEU	4.1
1	I	324	VAL	4.1
1	J	235	LEU	4.1
1	E	334	ALA	4.0
1	J	319	ILE	4.0
1	C	736	LEU	4.0
1	I	450	GLN	4.0
1	J	457	GLN	4.0
1	J	499	SER	4.0
1	D	502	THR	4.0
1	G	450	GLN	4.0
1	C	220	GLY	4.0
1	A	453	SER	4.0
1	B	453	SER	4.0
1	J	628	HIS	4.0
1	F	325	THR	4.0
1	H	327	ASN	4.0
1	G	343	VAL	4.0
1	E	556	ASP	3.9
1	A	326	THR	3.9
1	D	705	TYR	3.9
1	J	529	ASP	3.9
1	G	584	PHE	3.9
1	H	269	ASN	3.9
1	E	333	ILE	3.9
1	G	219	ASP	3.9
1	H	532	ASP	3.9
1	D	235	LEU	3.9
1	C	391	SER	3.9
1	H	330	VAL	3.9
1	J	330	VAL	3.9
1	G	458	ASN	3.9
1	I	704	ASN	3.9
1	D	532	ASP	3.9
1	G	223	ASN	3.8
1	J	253	ASN	3.8
1	G	517	ILE	3.8
1	C	244	THR	3.8
1	E	229	HIS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	691	ASN	3.8
1	G	556	ASP	3.8
1	I	219	ASP	3.8
1	J	333	ILE	3.8
1	J	312	LEU	3.8
1	J	532	ASP	3.8
1	I	229	HIS	3.8
1	I	329	GLY	3.8
1	F	460	ASP	3.8
1	C	265	THR	3.8
1	E	325	THR	3.8
1	G	244	THR	3.8
1	J	387	ALA	3.8
1	F	529	ASP	3.8
1	G	237	ASP	3.8
1	G	494	THR	3.7
1	J	713	PHE	3.7
1	B	323	GLU	3.7
1	G	227	ASN	3.7
1	E	388	VAL	3.7
1	I	232	SER	3.7
1	I	243	SER	3.7
1	I	312	LEU	3.7
1	B	705	TYR	3.7
1	E	493	LYS	3.7
1	G	265	THR	3.7
1	D	546	GLU	3.7
1	E	312	LEU	3.7
1	A	457	GLN	3.7
1	H	451	ASN	3.7
1	G	492	THR	3.7
1	I	325	THR	3.7
1	A	229	HIS	3.7
1	J	377	GLY	3.7
1	J	670	PHE	3.7
1	I	736	LEU	3.7
1	J	364	PRO	3.7
1	A	502	THR	3.6
1	B	324	VAL	3.6
1	I	582	VAL	3.6
1	E	706	ALA	3.6
1	A	667	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	317	PHE	3.6
1	D	704	ASN	3.6
1	C	325	THR	3.6
1	D	331	THR	3.6
1	C	547	SER	3.6
1	G	709	ALA	3.6
1	J	360	GLN	3.6
1	J	726	PRO	3.6
1	D	710	ASN	3.6
1	J	290	CYS	3.6
1	H	323	GLU	3.6
1	J	489	VAL	3.6
1	H	264	SER	3.6
1	I	493	LYS	3.6
1	J	279	PRO	3.6
1	A	327	ASN	3.6
1	C	498	ASN	3.6
1	B	546	GLU	3.6
1	J	273	TYR	3.6
1	G	665	THR	3.6
1	H	325	THR	3.6
1	I	326	THR	3.6
1	C	544	GLY	3.6
1	B	458	ASN	3.6
1	I	641	LYS	3.5
1	A	705	TYR	3.5
1	C	388	VAL	3.5
1	I	331	THR	3.5
1	J	725	ARG	3.5
1	F	220	GLY	3.5
1	H	506	ALA	3.5
1	F	229	HIS	3.5
1	E	323	GLU	3.5
1	D	264	SER	3.5
1	I	220	GLY	3.5
1	J	305	TRP	3.5
1	C	532	ASP	3.5
1	C	704	ASN	3.5
1	E	704	ASN	3.5
1	E	398	TYR	3.5
1	A	656	ALA	3.5
1	E	660	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	222	GLY	3.5
1	H	329	GLY	3.5
1	J	268	SER	3.5
1	J	571	PRO	3.5
1	G	641	LYS	3.5
1	F	323	GLU	3.5
1	D	457	GLN	3.5
1	J	243	SER	3.5
1	J	401	SER	3.5
1	J	601	ALA	3.5
1	C	223	ASN	3.4
1	C	492	THR	3.4
1	H	502	THR	3.4
1	E	702	THR	3.4
1	B	263	ALA	3.4
1	E	243	SER	3.4
1	D	229	HIS	3.4
1	J	376	TYR	3.4
1	I	564	GLU	3.4
1	C	219	ASP	3.4
1	G	328	ASP	3.4
1	J	458	ASN	3.4
1	E	736	LEU	3.4
1	I	235	LEU	3.4
1	D	329	GLY	3.4
1	F	232	SER	3.4
1	F	328	ASP	3.4
1	J	696	ASN	3.4
1	C	502	THR	3.4
1	D	702	THR	3.4
1	E	699	VAL	3.4
1	D	220	GLY	3.4
1	F	217	GLY	3.4
1	E	691	ASN	3.3
1	E	332	THR	3.3
1	J	439	ILE	3.3
1	J	469	ALA	3.3
1	J	709	ALA	3.3
1	G	499	SER	3.3
1	I	264	SER	3.3
1	I	538	SER	3.3
1	E	535	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	534	PHE	3.3
1	D	641	LYS	3.3
1	I	269	ASN	3.3
1	D	494	THR	3.3
1	F	326	THR	3.3
1	J	338	THR	3.3
1	A	266	GLY	3.3
1	G	263	ALA	3.3
1	I	523	ALA	3.3
1	E	490	SER	3.3
1	J	262	SER	3.3
1	J	667	PHE	3.3
1	G	483	CYS	3.3
1	E	235	LEU	3.3
1	H	235	LEU	3.3
1	E	628	HIS	3.3
1	G	221	VAL	3.3
1	B	494	THR	3.3
1	E	470	GLY	3.3
1	G	719	GLY	3.3
1	H	549	GLY	3.3
1	J	220	GLY	3.3
1	J	668	ALA	3.3
1	B	704	ASN	3.3
1	D	458	ASN	3.3
1	F	704	ASN	3.3
1	H	691	ASN	3.3
1	G	238	ARG	3.3
1	J	644	PRO	3.3
1	B	397	GLU	3.3
1	B	326	THR	3.3
1	E	244	THR	3.3
1	J	502	THR	3.3
1	J	579	THR	3.3
1	J	702	THR	3.3
1	J	727	ILE	3.3
1	D	660	ALA	3.3
1	J	493	LYS	3.3
1	J	680	SER	3.2
1	J	501	PHE	3.2
1	F	556	ASP	3.2
1	H	556	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	556	ASP	3.2
1	J	313	ASN	3.2
1	J	640	LEU	3.2
1	J	679	VAL	3.2
1	F	579	THR	3.2
1	J	384	GLY	3.2
1	G	493	LYS	3.2
1	E	457	GLN	3.2
1	E	355	LEU	3.2
1	J	395	CYS	3.2
1	C	221	VAL	3.2
1	I	459	LYS	3.2
1	I	501	PHE	3.2
1	C	235	LEU	3.2
1	E	300	LEU	3.2
1	H	458	ASN	3.2
1	J	227	ASN	3.2
1	J	302	ASN	3.2
1	F	407	GLY	3.2
1	I	573	ALA	3.2
1	J	525	ALA	3.2
1	J	320	GLN	3.2
1	C	503	TRP	3.2
1	F	587	SER	3.2
1	J	283	PHE	3.2
1	J	587	SER	3.2
1	I	443	LEU	3.2
1	J	404	LEU	3.2
1	J	437	PRO	3.2
1	J	613	TYR	3.2
1	F	494	THR	3.2
1	J	449	THR	3.2
1	F	263	ALA	3.1
1	I	656	ALA	3.1
1	I	660	ALA	3.1
1	J	224	ALA	3.1
1	E	360	GLN	3.1
1	G	421	PHE	3.1
1	J	410	PHE	3.1
1	J	619	TRP	3.1
1	J	590	ASP	3.1
1	F	266	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	321	VAL	3.1
1	G	536	PRO	3.1
1	J	631	PRO	3.1
1	D	736	LEU	3.1
1	H	704	ASN	3.1
1	I	302	ASN	3.1
1	I	221	VAL	3.1
1	E	683	ILE	3.1
1	C	584	PHE	3.1
1	E	399	PHE	3.1
1	I	316	LEU	3.1
1	J	264	SER	3.1
1	J	461	LEU	3.1
1	G	247	TRP	3.1
1	C	451	ASN	3.1
1	J	269	ASN	3.1
1	H	220	GLY	3.1
1	J	549	GLY	3.1
1	J	388	VAL	3.1
1	J	398	TYR	3.1
1	F	450	GLN	3.1
1	A	235	LEU	3.1
1	B	328	ASP	3.1
1	E	622	ILE	3.1
1	E	331	THR	3.0
1	H	232	SER	3.0
1	H	223	ASN	3.0
1	D	341	VAL	3.0
1	I	388	VAL	3.0
1	A	265	THR	3.0
1	B	522	THR	3.0
1	G	279	PRO	3.0
1	J	400	PRO	3.0
1	J	669	SER	3.0
1	B	451	ASN	3.0
1	G	498	ASN	3.0
1	I	223	ASN	3.0
1	J	226	GLY	3.0
1	D	388	VAL	3.0
1	D	450	GLN	3.0
1	E	324	VAL	3.0
1	G	489	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	301	ILE	3.0
1	J	711	VAL	3.0
1	F	665	THR	3.0
1	D	267	ALA	3.0
1	E	559	MET	3.0
1	I	484	TYR	3.0
1	J	509	TYR	3.0
1	J	716	ASP	3.0
1	D	230	CYS	3.0
1	J	483	CYS	3.0
1	I	587	SER	3.0
1	C	570	ASN	3.0
1	B	582	VAL	3.0
1	G	246	THR	3.0
1	H	546	GLU	3.0
1	J	724	PRO	3.0
1	B	641	LYS	3.0
1	J	296	ASP	3.0
1	F	588	SER	3.0
1	E	320	GLN	3.0
1	A	671	ILE	2.9
1	G	319	ILE	2.9
1	E	661	GLU	2.9
1	J	661	GLU	2.9
1	J	244	THR	2.9
1	C	422	HIS	2.9
1	C	257	TYR	2.9
1	F	219	ASP	2.9
1	E	232	SER	2.9
1	H	320	GLN	2.9
1	J	306	GLY	2.9
1	J	539	GLY	2.9
1	E	542	ILE	2.9
1	B	388	VAL	2.9
1	F	564	GLU	2.9
1	G	711	VAL	2.9
1	H	332	THR	2.9
1	B	525	ALA	2.9
1	G	668	ALA	2.9
1	I	525	ALA	2.9
1	J	550	ALA	2.9
1	E	503	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	305	TRP	2.9
1	C	396	LEU	2.9
1	J	337	LEU	2.9
1	B	460	ASP	2.9
1	I	460	ASP	2.9
1	J	416	PHE	2.9
1	A	220	GLY	2.9
1	B	269	ASN	2.9
1	C	327	ASN	2.9
1	E	266	GLY	2.9
1	E	513	GLY	2.9
1	J	407	GLY	2.9
1	H	324	VAL	2.9
1	J	359	HIS	2.9
1	C	326	THR	2.9
1	B	536	PRO	2.9
1	F	506	ALA	2.9
1	J	707	LYS	2.9
1	J	701	TYR	2.9
1	C	546	GLU	2.9
1	G	424	SER	2.9
1	G	703	SER	2.9
1	I	563	GLU	2.9
1	J	546	GLU	2.9
1	D	324	VAL	2.9
1	E	494	THR	2.9
1	E	645	PRO	2.9
1	I	589	THR	2.9
1	J	326	THR	2.9
1	J	300	LEU	2.9
1	J	443	LEU	2.9
1	J	602	LEU	2.9
1	B	219	ASP	2.9
1	B	562	ASP	2.9
1	E	429	GLN	2.9
1	J	421	PHE	2.9
1	C	710	ASN	2.8
1	G	311	ARG	2.8
1	G	669	SER	2.8
1	J	254	ASN	2.8
1	J	691	ASN	2.8
1	J	567	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	711	VAL	2.8
1	D	326	THR	2.8
1	J	494	THR	2.8
1	J	672	THR	2.8
1	D	263	ALA	2.8
1	G	548	ALA	2.8
1	J	479	LEU	2.8
1	D	503	TRP	2.8
1	J	450	GLN	2.8
1	J	460	ASP	2.8
1	F	563	GLU	2.8
1	I	236	GLY	2.8
1	D	373	ILE	2.8
1	D	551	SER	2.8
1	E	313	ASN	2.8
1	E	392	SER	2.8
1	J	526	SER	2.8
1	J	551	SER	2.8
1	J	618	ILE	2.8
1	B	221	VAL	2.8
1	C	654	VAL	2.8
1	I	699	VAL	2.8
1	E	603	PRO	2.8
1	D	244	THR	2.8
1	D	492	THR	2.8
1	E	246	THR	2.8
1	G	502	THR	2.8
1	J	358	ALA	2.8
1	B	316	LEU	2.8
1	E	555	LEU	2.8
1	G	396	LEU	2.8
1	J	396	LEU	2.8
1	G	459	LYS	2.8
1	C	361	GLY	2.8
1	E	394	TYR	2.8
1	E	674	TYR	2.8
1	J	444	TYR	2.8
1	G	500	ASN	2.8
1	G	717	ASN	2.8
1	E	365	PRO	2.8
1	B	574	THR	2.8
1	D	706	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	326	THR	2.8
1	G	504	THR	2.8
1	J	325	THR	2.8
1	F	235	LEU	2.8
1	I	397	GLU	2.8
1	F	311	ARG	2.8
1	I	237	ASP	2.8
1	J	607	TRP	2.8
1	E	273	TYR	2.8
1	E	319	ILE	2.8
1	J	517	ILE	2.8
1	C	669	SER	2.8
1	D	496	ASN	2.8
1	F	451	ASN	2.8
1	G	691	ASN	2.8
1	J	717	ASN	2.8
1	C	341	VAL	2.8
1	G	724	PRO	2.8
1	I	726	PRO	2.8
1	E	461	LEU	2.8
1	G	469	ALA	2.8
1	F	562	ASP	2.8
1	F	628	HIS	2.8
1	E	314	PHE	2.8
1	I	549	GLY	2.7
1	J	594	GLY	2.7
1	E	223	ASN	2.7
1	J	234	TRP	2.7
1	J	425	TYR	2.7
1	C	357	SER	2.7
1	H	547	SER	2.7
1	J	547	SER	2.7
1	C	331	THR	2.7
1	I	338	THR	2.7
1	J	434	LEU	2.7
1	J	315	LYS	2.7
1	J	346	ASP	2.7
1	D	266	GLY	2.7
1	E	407	GLY	2.7
1	J	260	ILE	2.7
1	C	302	ASN	2.7
1	E	497	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	655	PRO	2.7
1	F	657	ASN	2.7
1	I	588	SER	2.7
1	J	297	TRP	2.7
1	J	321	VAL	2.7
1	J	721	TYR	2.7
1	D	555	LEU	2.7
1	A	660	ALA	2.7
1	A	666	LYS	2.7
1	C	641	LYS	2.7
1	G	340	THR	2.7
1	C	323	GLU	2.7
1	J	429	GLN	2.7
1	J	673	GLN	2.7
1	G	422	HIS	2.7
1	D	362	CYS	2.7
1	G	532	ASP	2.7
1	B	637	GLY	2.7
1	C	670	PHE	2.7
1	E	283	PHE	2.7
1	F	501	PHE	2.7
1	G	713	PHE	2.7
1	I	539	GLY	2.7
1	J	399	PHE	2.7
1	J	543	PHE	2.7
1	I	517	ILE	2.7
1	I	653	PRO	2.7
1	D	691	ASN	2.7
1	B	239	VAL	2.7
1	D	268	SER	2.7
1	F	221	VAL	2.7
1	J	464	SER	2.7
1	J	596	VAL	2.7
1	G	282	TYR	2.7
1	H	736	LEU	2.7
1	J	355	LEU	2.7
1	J	478	TRP	2.7
1	J	641	LYS	2.7
1	B	568	ALA	2.7
1	C	506	ALA	2.7
1	E	469	ALA	2.7
1	G	332	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	334	ALA	2.7
1	J	561	THR	2.7
1	C	564	GLU	2.7
1	D	440	ASP	2.7
1	I	562	ASP	2.7
1	E	670	PHE	2.7
1	G	412	PHE	2.7
1	B	223	ASN	2.7
1	E	533	LYS	2.7
1	F	734	ARG	2.7
1	I	434	LEU	2.7
1	J	736	LEU	2.7
1	C	672	THR	2.7
1	C	706	ALA	2.7
1	I	263	ALA	2.7
1	I	478	TRP	2.7
1	I	503	TRP	2.7
1	I	702	THR	2.7
1	J	575	GLU	2.7
1	J	664	ALA	2.7
1	J	676	THR	2.7
1	C	628	HIS	2.7
1	I	624	HIS	2.7
1	H	616	GLY	2.6
1	E	501	PHE	2.6
1	I	591	PRO	2.6
1	J	468	PRO	2.6
1	A	269	ASN	2.6
1	F	498	ASN	2.6
1	G	269	ASN	2.6
1	H	710	ASN	2.6
1	J	710	ASN	2.6
1	F	239	VAL	2.6
1	J	239	VAL	2.6
1	E	680	SER	2.6
1	G	262	SER	2.6
1	J	385	SER	2.6
1	B	722	THR	2.6
1	F	331	THR	2.6
1	F	568	ALA	2.6
1	J	714	THR	2.6
1	H	628	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	532	ASP	2.6
1	E	460	ASP	2.6
1	I	266	GLY	2.6
1	I	543	PHE	2.6
1	J	367	PRO	2.6
1	J	518	ILE	2.6
1	J	605	MET	2.6
1	C	483	CYS	2.6
1	D	269	ASN	2.6
1	I	253	ASN	2.6
1	J	316	LEU	2.6
1	J	511	LEU	2.6
1	J	519	ASN	2.6
1	F	341	VAL	2.6
1	J	397	GLU	2.6
1	E	538	SER	2.6
1	I	262	SER	2.6
1	I	516	SER	2.6
1	E	492	THR	2.6
1	E	593	THR	2.6
1	G	660	ALA	2.6
1	H	326	THR	2.6
1	J	406	THR	2.6
1	A	503	TRP	2.6
1	F	384	GLY	2.6
1	J	536	PRO	2.6
1	F	667	PHE	2.6
1	G	501	PHE	2.6
1	I	541	MET	2.6
1	C	511	LEU	2.6
1	F	313	ASN	2.6
1	F	580	VAL	2.6
1	G	651	ASN	2.6
1	J	221	VAL	2.6
1	C	551	SER	2.6
1	A	494	THR	2.6
1	C	332	THR	2.6
1	F	660	ALA	2.6
1	J	248	ALA	2.6
1	J	592	ALA	2.6
1	E	249	LEU	2.6
1	G	736	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	223	ASN	2.6
1	I	451	ASN	2.6
1	I	673	GLN	2.6
1	D	347	SER	2.6
1	E	592	ALA	2.6
1	F	499	SER	2.6
1	I	339	SER	2.6
1	J	632	SER	2.6
1	C	714	THR	2.6
1	H	492	THR	2.6
1	I	332	THR	2.6
1	G	725	ARG	2.5
1	B	521	GLY	2.5
1	E	296	ASP	2.5
1	J	655	PRO	2.5
1	C	421	PHE	2.5
1	H	397	GLU	2.5
1	I	670	PHE	2.5
1	B	691	ASN	2.5
1	C	711	VAL	2.5
1	F	519	ASN	2.5
1	H	540	VAL	2.5
1	I	313	ASN	2.5
1	C	668	ALA	2.5
1	F	230	CYS	2.5
1	C	553	THR	2.5
1	G	574	THR	2.5
1	I	242	THR	2.5
1	I	494	THR	2.5
1	I	593	THR	2.5
1	J	277	SER	2.5
1	J	665	THR	2.5
1	B	333	ILE	2.5
1	C	671	ILE	2.5
1	G	297	TRP	2.5
1	E	546	GLU	2.5
1	C	462	LEU	2.5
1	I	363	LEU	2.5
1	I	700	GLN	2.5
1	C	567	LYS	2.5
1	D	580	VAL	2.5
1	E	436	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	388	VAL	2.5
1	I	580	VAL	2.5
1	E	668	ALA	2.5
1	F	664	ALA	2.5
1	I	548	ALA	2.5
1	J	263	ALA	2.5
1	B	332	THR	2.5
1	E	278	THR	2.5
1	E	672	THR	2.5
1	F	504	THR	2.5
1	G	464	SER	2.5
1	G	589	THR	2.5
1	H	331	THR	2.5
1	D	725	ARG	2.5
1	G	273	TYR	2.5
1	I	275	GLY	2.5
1	C	626	ASP	2.5
1	C	716	ASP	2.5
1	C	260	ILE	2.5
1	J	542	ILE	2.5
1	E	478	TRP	2.5
1	B	501	PHE	2.5
1	G	461	LEU	2.5
1	B	229	HIS	2.5
1	A	451	ASN	2.5
1	B	341	VAL	2.5
1	D	628	HIS	2.5
1	E	580	VAL	2.5
1	I	489	VAL	2.5
1	H	709	ALA	2.5
1	J	299	ARG	2.5
1	A	492	THR	2.5
1	B	625	THR	2.5
1	C	586	SER	2.5
1	D	232	SER	2.5
1	D	547	SER	2.5
1	E	338	THR	2.5
1	E	464	SER	2.5
1	G	339	SER	2.5
1	H	357	SER	2.5
1	I	504	THR	2.5
1	I	676	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	339	SER	2.5
1	C	724	PRO	2.5
1	D	323	GLU	2.5
1	I	544	GLY	2.5
1	J	578	GLY	2.5
1	B	369	ASP	2.5
1	G	414	TYR	2.5
1	B	671	ILE	2.5
1	I	566	ILE	2.5
1	J	284	ASP	2.5
1	F	648	LEU	2.5
1	G	337	LEU	2.5
1	E	662	PHE	2.5
1	G	366	PHE	2.5
1	J	255	HIS	2.5
1	C	496	ASN	2.5
1	E	465	ARG	2.5
1	E	498	ASN	2.5
1	J	238	ARG	2.5
1	B	426	ALA	2.5
1	B	709	ALA	2.5
1	D	548	ALA	2.5
1	G	525	ALA	2.5
1	E	411	THR	2.5
1	J	233	THR	2.5
1	J	553	THR	2.5
1	J	692	SER	2.5
1	F	735	PRO	2.4
1	I	230	CYS	2.4
1	I	290	CYS	2.4
1	C	348	GLU	2.4
1	C	389	GLY	2.4
1	J	481	GLY	2.4
1	J	544	GLY	2.4
1	E	257	TYR	2.4
1	E	701	TYR	2.4
1	E	712	ASP	2.4
1	F	237	ASP	2.4
1	I	284	ASP	2.4
1	J	328	ASP	2.4
1	I	381	LEU	2.4
1	J	687	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	317	PHE	2.4
1	E	412	PHE	2.4
1	E	667	PHE	2.4
1	J	285	PHE	2.4
1	J	534	PHE	2.4
1	C	239	VAL	2.4
1	D	221	VAL	2.4
1	B	248	ALA	2.4
1	B	267	ALA	2.4
1	C	380	THR	2.4
1	C	574	THR	2.4
1	H	504	THR	2.4
1	J	278	THR	2.4
1	I	735	PRO	2.4
1	J	653	PRO	2.4
1	A	397	GLU	2.4
1	I	661	GLU	2.4
1	F	483	CYS	2.4
1	I	222	GLY	2.4
1	B	727	ILE	2.4
1	I	671	ILE	2.4
1	J	671	ILE	2.4
1	E	350	GLN	2.4
1	G	360	GLN	2.4
1	G	613	TYR	2.4
1	J	350	GLN	2.4
1	J	378	TYR	2.4
1	J	486	GLN	2.4
1	J	720	LEU	2.4
1	D	501	PHE	2.4
1	E	344	PHE	2.4
1	H	501	PHE	2.4
1	B	503	TRP	2.4
1	C	324	VAL	2.4
1	G	354	VAL	2.4
1	I	458	ASN	2.4
1	I	496	ASN	2.4
1	J	642	ASN	2.4
1	B	548	ALA	2.4
1	H	665	THR	2.4
1	B	551	SER	2.4
1	E	588	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	661	GLU	2.4
1	G	323	GLU	2.4
1	J	617	PRO	2.4
1	J	689	LYS	2.4
1	H	266	GLY	2.4
1	E	369	ASP	2.4
1	F	319	ILE	2.4
1	G	333	ILE	2.4
1	G	518	ILE	2.4
1	B	235	LEU	2.4
1	G	479	LEU	2.4
1	I	438	LEU	2.4
1	G	378	TYR	2.4
1	I	273	TYR	2.4
1	I	274	PHE	2.4
1	E	489	VAL	2.4
1	H	580	VAL	2.4
1	A	691	ASN	2.4
1	E	253	ASN	2.4
1	E	451	ASN	2.4
1	E	477	ASN	2.4
1	J	512	ASN	2.4
1	E	234	TRP	2.4
1	E	554	ALA	2.4
1	G	478	TRP	2.4
1	J	503	TRP	2.4
1	B	246	THR	2.4
1	C	522	THR	2.4
1	I	374	PRO	2.4
1	E	703	SER	2.4
1	F	547	SER	2.4
1	I	345	SER	2.4
1	J	467	SER	2.4
1	E	549	GLY	2.4
1	H	281	GLY	2.4
1	J	627	GLY	2.4
1	E	671	ILE	2.4
1	A	628	HIS	2.4
1	E	648	LEU	2.4
1	F	736	LEU	2.4
1	H	396	LEU	2.4
1	I	720	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	237	ASP	2.4
1	A	543	PHE	2.4
1	B	713	PHE	2.4
1	F	701	TYR	2.4
1	E	679	VAL	2.4
1	H	388	VAL	2.4
1	E	696	ASN	2.4
1	F	269	ASN	2.4
1	J	304	ASN	2.4
1	B	581	ALA	2.4
1	D	469	ALA	2.4
1	E	387	ALA	2.4
1	F	641	LYS	2.4
1	H	706	ALA	2.4
1	I	709	ALA	2.4
1	J	533	LYS	2.4
1	G	723	GLU	2.4
1	B	702	THR	2.3
1	D	665	THR	2.3
1	J	241	THR	2.3
1	C	268	SER	2.3
1	C	464	SER	2.3
1	E	391	SER	2.3
1	H	389	GLY	2.3
1	J	466	GLY	2.3
1	G	249	LEU	2.3
1	H	316	LEU	2.3
1	I	333	ILE	2.3
1	J	514	ARG	2.3
1	C	312	LEU	2.3
1	C	529	ASP	2.3
1	F	555	LEU	2.3
1	J	646	GLN	2.3
1	I	712	ASP	2.3
1	E	362	CYS	2.3
1	J	524	MET	2.3
1	C	292	PHE	2.3
1	D	398	TYR	2.3
1	G	399	PHE	2.3
1	I	421	PHE	2.3
1	I	444	TYR	2.3
1	I	535	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	257	TYR	2.3
1	B	666	LYS	2.3
1	G	239	VAL	2.3
1	H	341	VAL	2.3
1	C	318	ASN	2.3
1	C	552	ASN	2.3
1	D	500	ASN	2.3
1	E	304	ASN	2.3
1	G	313	ASN	2.3
1	J	271	ASN	2.3
1	J	657	ASN	2.3
1	H	548	ALA	2.3
1	E	400	PRO	2.3
1	E	729	THR	2.3
1	I	672	THR	2.3
1	J	242	THR	2.3
1	B	708	SER	2.3
1	C	243	SER	2.3
1	C	588	SER	2.3
1	E	547	SER	2.3
1	J	390	ARG	2.3
1	B	450	GLN	2.3
1	C	618	ILE	2.3
1	C	673	GLN	2.3
1	E	673	GLN	2.3
1	I	319	ILE	2.3
1	J	462	LEU	2.3
1	J	530	ASP	2.3
1	J	562	ASP	2.3
1	J	372	MET	2.3
1	E	315	LYS	2.3
1	F	534	PHE	2.3
1	G	230	CYS	2.3
1	G	577	PHE	2.3
1	E	572	VAL	2.3
1	G	509	TYR	2.3
1	D	563	GLU	2.3
1	C	510	ASN	2.3
1	E	710	ASN	2.3
1	G	271	ASN	2.3
1	E	568	ALA	2.3
1	E	573	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	374	PRO	2.3
1	B	331	THR	2.3
1	C	449	THR	2.3
1	E	589	THR	2.3
1	H	449	THR	2.3
1	C	734	ARG	2.3
1	J	576	ARG	2.3
1	C	636	GLY	2.3
1	E	220	GLY	2.3
1	F	685	TRP	2.3
1	E	566	ILE	2.3
1	E	602	LEU	2.3
1	F	671	ILE	2.3
1	H	462	LEU	2.3
1	B	296	ASP	2.3
1	B	530	ASP	2.3
1	C	432	ASP	2.3
1	E	605	MET	2.3
1	F	712	ASP	2.3
1	G	296	ASP	2.3
1	A	398	TYR	2.3
1	A	580	VAL	2.3
1	F	257	TYR	2.3
1	G	580	VAL	2.3
1	E	496	ASN	2.3
1	G	520	PRO	2.3
1	G	718	ASN	2.3
1	J	286	ASN	2.3
1	J	554	ALA	2.3
1	A	665	THR	2.3
1	B	714	THR	2.3
1	C	486	GLN	2.3
1	F	639	GLY	2.3
1	G	628	HIS	2.3
1	H	450	GLN	2.3
1	I	281	GLY	2.3
1	I	521	GLY	2.3
1	J	608	GLN	2.3
1	E	587	SER	2.3
1	I	507	SER	2.3
1	E	381	LEU	2.3
1	G	301	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	312	LEU	2.3
1	J	622	ILE	2.3
1	E	562	ASP	2.3
1	F	296	ASP	2.3
1	F	666	LYS	2.3
1	H	459	LYS	2.3
1	B	661	GLU	2.3
1	C	501	PHE	2.3
1	E	421	PHE	2.3
1	G	661	GLU	2.3
1	H	535	PHE	2.3
1	H	584	PHE	2.3
1	H	661	GLU	2.3
1	J	412	PHE	2.3
1	J	682	GLU	2.3
1	A	341	VAL	2.3
1	B	540	VAL	2.3
1	F	324	VAL	2.3
1	B	362	CYS	2.3
1	C	445	TYR	2.3
1	C	484	TYR	2.3
1	E	269	ASN	2.2
1	E	510	ASN	2.2
1	E	581	ALA	2.2
1	G	335	ASN	2.2
1	H	620	ALA	2.2
1	J	223	ASN	2.2
1	B	504	THR	2.2
1	E	242	THR	2.2
1	G	449	THR	2.2
1	E	298	GLN	2.2
1	A	261	SER	2.2
1	C	517	ILE	2.2
1	D	459	LYS	2.2
1	D	516	SER	2.2
1	G	373	ILE	2.2
1	J	261	SER	2.2
1	B	619	TRP	2.2
1	G	712	ASP	2.2
1	I	297	TRP	2.2
1	A	661	GLU	2.2
1	J	563	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	584	PHE	2.2
1	G	463	PHE	2.2
1	I	412	PHE	2.2
1	J	307	PHE	2.2
1	E	715	VAL	2.2
1	F	343	VAL	2.2
1	F	388	VAL	2.2
1	F	489	VAL	2.2
1	H	311	ARG	2.2
1	I	239	VAL	2.2
1	J	324	VAL	2.2
1	J	658	PRO	2.2
1	J	681	VAL	2.2
1	J	697	PRO	2.2
1	B	398	TYR	2.2
1	B	721	TYR	2.2
1	C	398	TYR	2.2
1	E	484	TYR	2.2
1	G	442	TYR	2.2
1	G	674	TYR	2.2
1	E	569	THR	2.2
1	J	332	THR	2.2
1	J	574	THR	2.2
1	J	589	THR	2.2
1	A	719	GLY	2.2
1	B	322	LYS	2.2
1	B	459	LYS	2.2
1	B	470	GLY	2.2
1	C	594	GLY	2.2
1	E	275	GLY	2.2
1	J	521	GLY	2.2
1	J	616	GLY	2.2
1	C	363	LEU	2.2
1	E	499	SER	2.2
1	G	385	SER	2.2
1	H	588	SER	2.2
1	H	669	SER	2.2
1	J	663	SER	2.2
1	F	546	GLU	2.2
1	G	245	ARG	2.2
1	J	463	PHE	2.2
1	C	617	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	367	PRO	2.2
1	E	617	PRO	2.2
1	G	644	PRO	2.2
1	H	221	VAL	2.2
1	I	468	PRO	2.2
1	A	267	ALA	2.2
1	C	271	ASN	2.2
1	C	717	ASN	2.2
1	E	601	ALA	2.2
1	F	706	ALA	2.2
1	I	498	ASN	2.2
1	J	335	ASN	2.2
1	J	477	ASN	2.2
1	J	718	ASN	2.2
1	B	353	TYR	2.2
1	C	350	GLN	2.2
1	C	527	HIS	2.2
1	G	276	TYR	2.2
1	H	398	TYR	2.2
1	I	398	TYR	2.2
1	J	624	HIS	2.2
1	C	504	THR	2.2
1	C	300	LEU	2.2
1	C	434	LEU	2.2
1	C	513	GLY	2.2
1	E	363	LEU	2.2
1	E	479	LEU	2.2
1	G	431	LEU	2.2
1	G	616	GLY	2.2
1	I	351	LEU	2.2
1	J	236	GLY	2.2
1	E	647	ILE	2.2
1	E	516	SER	2.2
1	H	499	SER	2.2
1	J	347	SER	2.2
1	E	346	ASP	2.2
1	B	418	GLU	2.2
1	C	280	TRP	2.2
1	G	503	TRP	2.2
1	G	730	ARG	2.2
1	C	577	PHE	2.2
1	E	285	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	662	PHE	2.2
1	G	670	PHE	2.2
1	C	343	VAL	2.2
1	I	596	VAL	2.2
1	J	572	VAL	2.2
1	C	469	ALA	2.2
1	I	469	ALA	2.2
1	I	717	ASN	2.2
1	J	426	ALA	2.2
1	J	498	ASN	2.2
1	J	510	ASN	2.2
1	E	486	GLN	2.2
1	B	257	TYR	2.2
1	B	589	THR	2.2
1	E	265	THR	2.2
1	E	579	THR	2.2
1	C	395	CYS	2.2
1	E	395	CYS	2.2
1	F	377	GLY	2.2
1	G	266	GLY	2.2
1	G	316	LEU	2.2
1	G	443	LEU	2.2
1	I	389	GLY	2.2
1	I	614	LEU	2.2
1	I	701	TYR	2.2
1	J	345	SER	2.2
1	E	659	PRO	2.2
1	E	393	PHE	2.2
1	F	371	PHE	2.2
1	J	310	LYS	2.2
1	B	580	VAL	2.1
1	C	572	VAL	2.1
1	E	321	VAL	2.1
1	C	360	GLN	2.1
1	D	320	GLN	2.1
1	E	372	MET	2.1
1	E	717	ASN	2.1
1	G	302	ASN	2.1
1	H	360	GLN	2.1
1	I	336	ASN	2.1
1	J	447	ASN	2.1
1	J	568	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	332	THR	2.1
1	A	714	THR	2.1
1	C	616	GLY	2.1
1	D	312	LEU	2.1
1	D	589	THR	2.1
1	F	511	LEU	2.1
1	J	381	LEU	2.1
1	J	732	LEU	2.1
1	C	442	TYR	2.1
1	C	433	ARG	2.1
1	E	723	GLU	2.1
1	G	277	SER	2.1
1	G	490	SER	2.1
1	H	299	ARG	2.1
1	J	405	ARG	2.1
1	J	418	GLU	2.1
1	B	556	ASP	2.1
1	E	225	SER	2.1
1	F	590	ASP	2.1
1	G	595	ASP	2.1
1	I	590	ASP	2.1
1	C	533	LYS	2.1
1	E	476	LYS	2.1
1	H	493	LYS	2.1
1	B	667	PHE	2.1
1	D	713	PHE	2.1
1	I	314	PHE	2.1
1	I	629	PHE	2.1
1	E	711	VAL	2.1
1	F	711	VAL	2.1
1	E	402	GLN	2.1
1	E	646	GLN	2.1
1	I	267	ALA	2.1
1	J	598	ALA	2.1
1	C	691	ASN	2.1
1	E	227	ASN	2.1
1	G	512	ASN	2.1
1	E	337	LEU	2.1
1	E	434	LEU	2.1
1	E	634	LEU	2.1
1	F	278	THR	2.1
1	F	316	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	355	LEU	2.1
1	I	677	GLY	2.1
1	D	333	ILE	2.1
1	E	727	ILE	2.1
1	E	252	TYR	2.1
1	E	390	ARG	2.1
1	G	425	TYR	2.1
1	I	690	GLU	2.1
1	J	394	TYR	2.1
1	B	587	SER	2.1
1	C	538	SER	2.1
1	E	495	ASP	2.1
1	E	663	SER	2.1
1	J	225	SER	2.1
1	J	392	SER	2.1
1	G	707	LYS	2.1
1	J	643	PRO	2.1
1	C	307	PHE	2.1
1	E	541	MET	2.1
1	E	543	PHE	2.1
1	G	307	PHE	2.1
1	G	427	HIS	2.1
1	I	577	PHE	2.1
1	J	577	PHE	2.1
1	J	599	MET	2.1
1	E	221	VAL	2.1
1	G	582	VAL	2.1
1	G	606	VAL	2.1
1	I	360	GLN	2.1
1	J	540	VAL	2.1
1	F	717	ASN	2.1
1	J	497	ASN	2.1
1	B	407	GLY	2.1
1	I	461	LEU	2.1
1	I	479	LEU	2.1
1	B	733	THR	2.1
1	F	722	THR	2.1
1	H	340	THR	2.1
1	I	513	GLY	2.1
1	I	522	THR	2.1
1	I	553	THR	2.1
1	J	652	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	323	GLU	2.1
1	E	684	GLU	2.1
1	E	551	SER	2.1
1	E	675	SER	2.1
1	F	716	ASP	2.1
1	J	626	ASP	2.1
1	E	364	PRO	2.1
1	B	527	HIS	2.1
1	G	537	MET	2.1
1	C	662	PHE	2.1
1	D	283	PHE	2.1
1	D	354	VAL	2.1
1	E	419	VAL	2.1
1	E	654	VAL	2.1
1	F	283	PHE	2.1
1	I	534	PHE	2.1
1	B	478	TRP	2.1
1	D	227	ASN	2.1
1	E	316	LEU	2.1
1	G	511	LEU	2.1
1	I	408	ASN	2.1
1	B	539	GLY	2.1
1	C	356	GLY	2.1
1	G	306	GLY	2.1
1	G	636	GLY	2.1
1	G	694	ARG	2.1
1	H	361	GLY	2.1
1	F	589	THR	2.1
1	H	564	GLU	2.1
1	J	531	GLU	2.1
1	H	319	ILE	2.1
1	J	647	ILE	2.1
1	C	545	LYS	2.1
1	D	493	LYS	2.1
1	E	567	LYS	2.1
1	J	476	LYS	2.1
1	B	276	TYR	2.1
1	F	530	ASP	2.1
1	E	430	SER	2.1
1	E	692	SER	2.1
1	F	586	SER	2.1
1	J	490	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	708	SER	2.1
1	C	597	HIS	2.1
1	G	272	HIS	2.1
1	E	259	GLN	2.0
1	F	360	GLN	2.0
1	B	535	PHE	2.0
1	F	370	VAL	2.0
1	J	580	VAL	2.0
1	J	715	VAL	2.0
1	C	601	ALA	2.0
1	C	660	ALA	2.0
1	E	287	ARG	2.0
1	I	554	ALA	2.0
1	J	267	ALA	2.0
1	J	311	ARG	2.0
1	A	704	ASN	2.0
1	B	434	LEU	2.0
1	B	736	LEU	2.0
1	E	379	LEU	2.0
1	F	434	LEU	2.0
1	G	318	ASN	2.0
1	G	602	LEU	2.0
1	E	348	GLU	2.0
1	J	565	GLU	2.0
1	J	719	GLY	2.0
1	B	579	THR	2.0
1	F	518	ILE	2.0
1	H	494	THR	2.0
1	I	260	ILE	2.0
1	I	545	LYS	2.0
1	J	411	THR	2.0
1	J	504	THR	2.0
1	B	268	SER	2.0
1	C	293	SER	2.0
1	C	587	SER	2.0
1	G	468	PRO	2.0
1	H	703	SER	2.0
1	I	367	PRO	2.0
1	J	480	PRO	2.0
1	C	599	MET	2.0
1	F	527	HIS	2.0
1	B	360	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	320	GLN	2.0
1	G	395	CYS	2.0
1	B	390	ARG	2.0
1	E	311	ARG	2.0
1	E	343	VAL	2.0
1	E	534	PHE	2.0
1	H	343	VAL	2.0
1	H	534	PHE	2.0
1	J	465	ARG	2.0
1	A	263	ALA	2.0
1	D	334	ALA	2.0
1	D	709	ALA	2.0
1	E	404	LEU	2.0
1	G	358	ALA	2.0
1	I	368	ALA	2.0
1	C	477	ASN	2.0
1	C	491	LYS	2.0
1	G	281	GLY	2.0
1	G	382	ASN	2.0
1	G	496	ASN	2.0
1	G	508	LYS	2.0
1	G	563	GLU	2.0
1	D	313	ASN	2.0
1	F	303	ASN	2.0
1	F	356	GLY	2.0
1	F	382	ASN	2.0
1	J	557	ASN	2.0
1	A	333	ILE	2.0
1	E	649	ILE	2.0
1	G	234	TRP	2.0
1	C	595	ASP	2.0
1	E	530	ASP	2.0
1	E	653	PRO	2.0
1	E	716	ASP	2.0
1	F	365	PRO	2.0
1	G	440	ASP	2.0
1	H	562	ASP	2.0
1	C	516	SER	2.0
1	E	444	TYR	2.0
1	E	509	TYR	2.0
1	G	289	HIS	2.0
1	I	509	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	703	SER	2.0
1	J	391	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CYT	H	738	8/8	0.60	0.32	63,67,68,70	0
3	CYT	F	738	8/8	0.65	0.27	63,67,68,70	0
3	CYT	E	738	8/8	0.65	0.25	63,67,68,70	0
3	CYT	D	738	8/8	0.66	0.28	63,67,68,70	0
2	ADE	F	737	10/10	0.70	0.32	78,81,82,83	0
3	CYT	B	739	8/8	0.70	0.25	63,67,68,70	0
3	CYT	C	738	8/8	0.71	0.27	63,67,68,70	0
3	CYT	J	738	8/8	0.71	0.23	63,67,68,70	0
3	CYT	I	738	8/8	0.77	0.23	63,67,68,70	0
3	CYT	B	738	8/8	0.79	0.22	63,67,68,70	0
2	ADE	E	737	10/10	0.79	0.29	78,81,82,83	0
3	CYT	A	738	8/8	0.79	0.26	63,67,68,70	0
2	ADE	I	737	10/10	0.80	0.25	78,81,82,83	0
2	ADE	D	737	10/10	0.82	0.25	78,81,82,83	0
2	ADE	C	737	10/10	0.83	0.24	78,81,82,83	0
2	ADE	A	737	10/10	0.84	0.21	78,81,82,83	0
2	ADE	J	737	10/10	0.84	0.24	78,81,82,83	0
2	ADE	G	737	10/10	0.84	0.24	78,81,82,83	0
2	ADE	H	737	10/10	0.85	0.21	78,81,82,83	0
2	ADE	B	737	10/10	0.86	0.20	78,81,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.