



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:55 PM UTC

PDB ID : 1ZYC / pdb_00001zyc
Title : Crystal Structure of eIF2alpha Protein Kinase GCN2: Wild-Type in Apo Form.
Authors : Padyana, A.K.; Qiu, H.; Roll-Mecak, A.; Hinnebusch, A.G.; Burley, S.K.
Deposited on : 2005-06-09
Resolution : 3.00 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
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

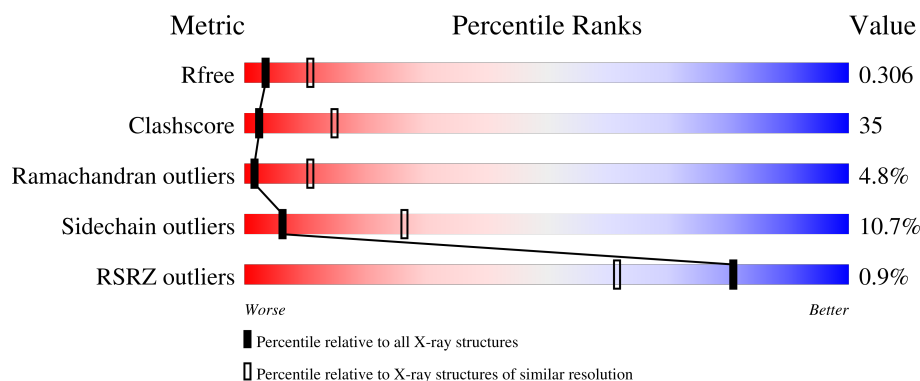
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	303	37% 40% 8% 14%
1	B	303	% 38% 36% 9% 16%
1	C	303	% 35% 44% 10% 11%
1	D	303	% 32% 41% 11% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8601 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 Serine/threonine-protein kinase GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	5	0	0
			2153	1378	375	391	9			
1	B	254	Total	C	N	O	S	0	0	0
			2091	1341	364	377	9			
1	C	271	Total	C	N	O	S	0	0	0
			2235	1435	388	403	9			
1	D	256	Total	C	N	O	S	0	0	0
			2108	1352	366	381	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	cloning artifact	UNP P15442
A	593	LEU	-	cloning artifact	UNP P15442
B	592	SER	-	cloning artifact	UNP P15442
B	593	LEU	-	cloning artifact	UNP P15442
C	592	SER	-	cloning artifact	UNP P15442
C	593	LEU	-	cloning artifact	UNP P15442
D	592	SER	-	cloning artifact	UNP P15442
D	593	LEU	-	cloning artifact	UNP P15442

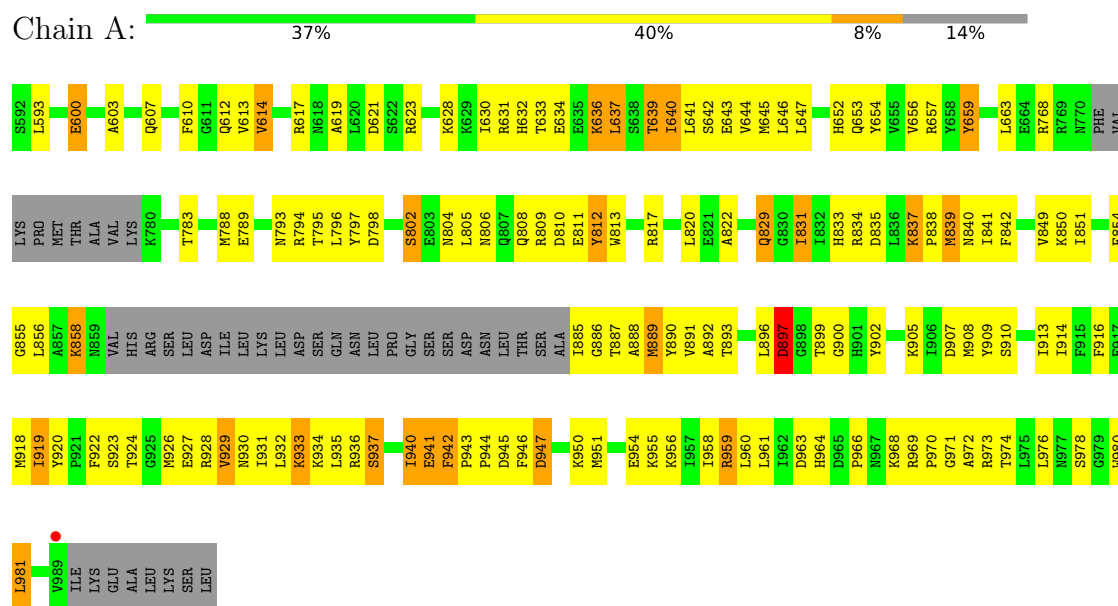
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	6	Total	O	0	0
			6	6		
2	C	5	Total	O	0	0
			5	5		

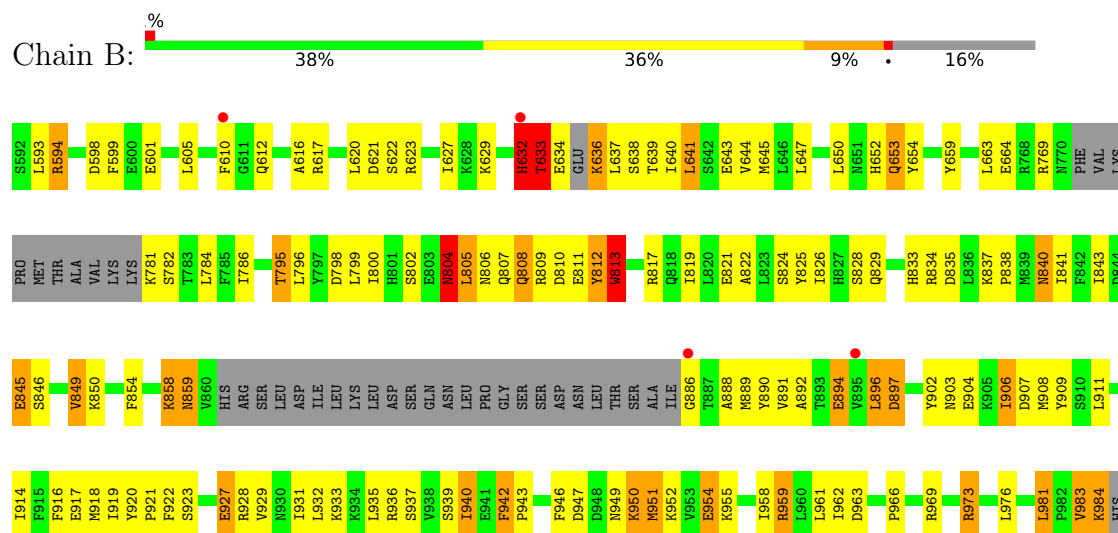
3 Residue-property plots

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: Serine/threonine-protein kinase GCN2

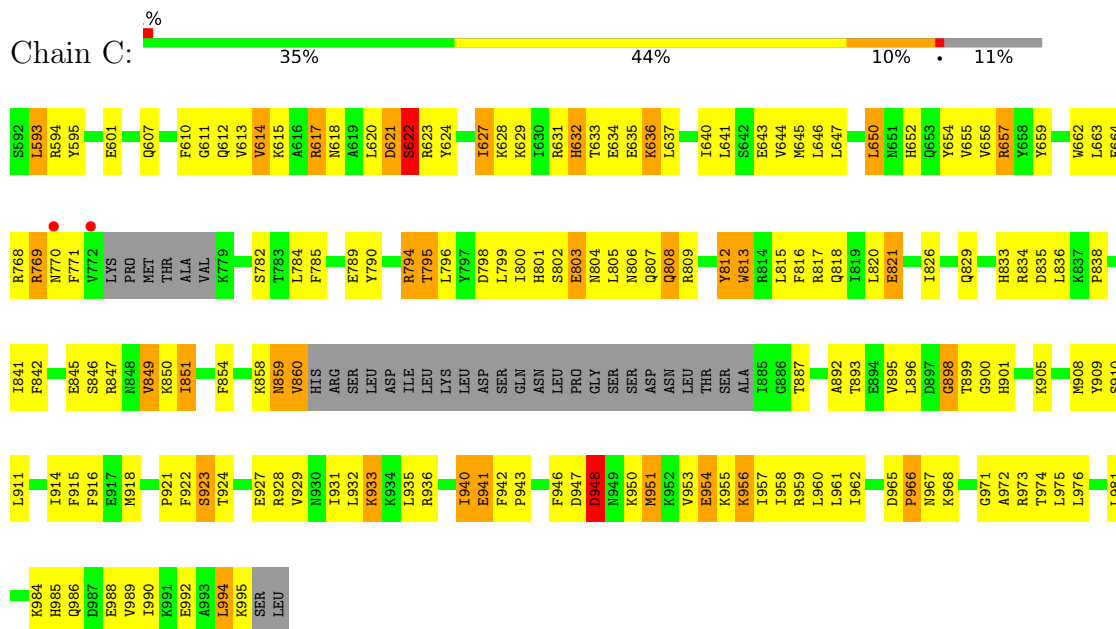


• Molecule 1: Serine/threonine-protein kinase GCN2

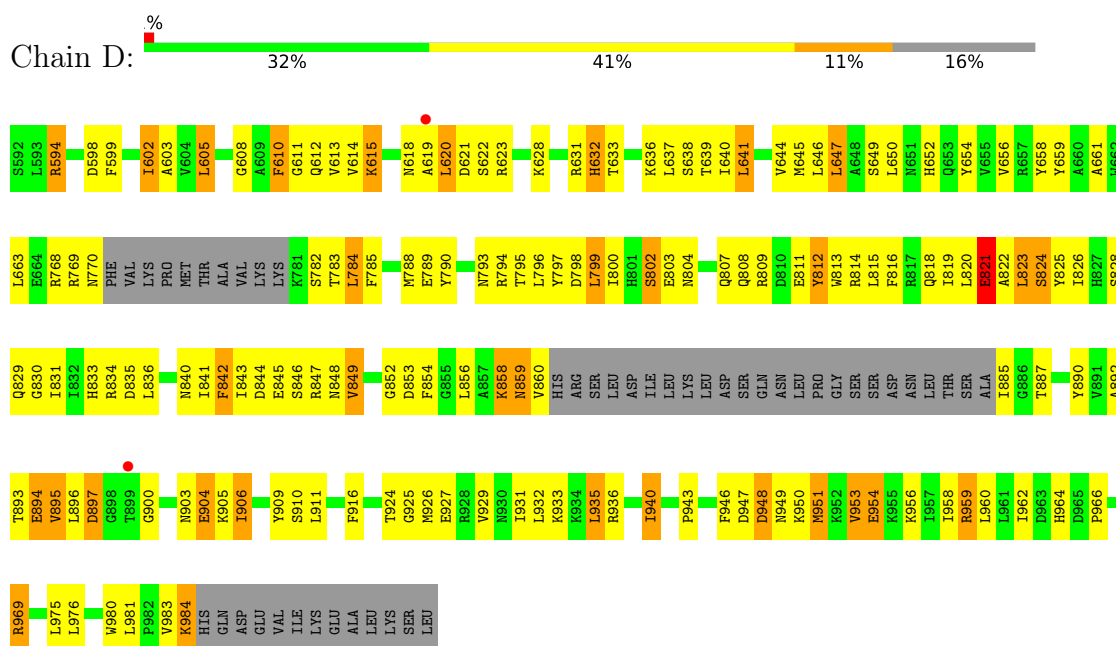


GLN
ASP
GLU
VAL
ILE
LYS
GLU
ALA
LYS
SER
LEU

• Molecule 1: Serine/threonine-protein kinase GCN2



• Molecule 1: Serine/threonine-protein kinase GCN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.89Å 95.70Å 175.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.99 – 3.00 41.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.6 (41.99-3.00) 94.5 (41.99-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.234 , 0.299 (Not available) , 0.306	Depositor DCC
R_{free} test set	652 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8601	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.32% 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

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	0.57	1/2196 (0.0%)	1.06	11/2956 (0.4%)
1	B	0.55	1/2132 (0.0%)	1.15	16/2869 (0.6%)
1	C	0.54	0/2279	1.01	11/3066 (0.4%)
1	D	0.56	0/2150	1.03	13/2895 (0.4%)
All	All	0.56	2/8757 (0.0%)	1.06	51/11786 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	632	HIS	CA-C	6.09	1.60	1.52
1	A	941	GLU	CA-C	5.83	1.59	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	THR	N-CA-C	17.94	141.84	108.65
1	A	659	TYR	N-CA-C	9.75	121.98	111.36
1	C	898	GLY	N-CA-C	-9.36	90.99	113.18
1	B	888	ALA	N-CA-C	-8.50	102.82	113.02
1	D	900	GLY	N-CA-C	-8.41	103.71	115.32
1	B	859	ASN	N-CA-C	7.64	127.07	110.80
1	A	919	ILE	N-CA-C	7.52	117.64	110.42
1	A	858	LYS	N-CA-C	7.46	126.68	110.80
1	B	599	PHE	N-CA-C	7.37	121.50	109.72
1	B	659	TYR	N-CA-C	7.36	118.99	110.97
1	D	796	LEU	N-CA-C	-7.34	103.28	111.28
1	B	594	ARG	N-CA-C	7.29	123.32	111.37
1	C	968	LYS	N-CA-C	-7.05	104.29	113.17
1	B	633	THR	CA-C-N	6.99	134.29	121.70
1	B	633	THR	C-N-CA	6.99	134.29	121.70
1	A	813	TRP	N-CA-C	-6.77	104.04	112.90
1	B	633	THR	CB-CA-C	-6.69	97.80	114.11
1	B	858	LYS	N-CA-C	6.68	121.63	107.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	627	ILE	N-CA-C	6.66	117.45	107.80
1	A	887	THR	N-CA-C	-6.54	104.15	111.28
1	A	956	LYS	N-CA-C	-6.48	104.30	111.36
1	A	793	ASN	N-CA-C	6.42	119.61	110.68
1	B	846	SER	N-CA-C	-6.41	103.76	113.89
1	B	641	LEU	N-CA-C	-6.36	103.65	111.40
1	D	799	LEU	N-CA-C	-6.35	104.79	112.54
1	B	620	LEU	N-CA-C	6.33	119.85	111.75
1	A	600	GLU	N-CA-C	-6.09	99.28	108.96
1	D	659	TYR	N-CA-C	6.01	117.70	111.03
1	C	657	ARG	N-CA-C	5.96	118.37	109.25
1	B	849	VAL	N-CA-C	5.90	118.25	109.17
1	A	900	GLY	N-CA-C	-5.88	106.02	115.08
1	A	842	PHE	N-CA-C	5.82	118.71	110.50
1	C	813	TRP	N-CA-C	-5.76	106.42	113.50
1	C	956	LYS	N-CA-C	-5.65	105.22	111.71
1	D	842	PHE	N-CA-C	5.63	117.96	110.53
1	D	943	PRO	CA-C-N	5.59	125.25	119.05
1	D	943	PRO	C-N-CA	5.59	125.25	119.05
1	C	650	LEU	N-CA-C	5.53	118.30	110.50
1	A	907	ASP	N-CA-C	-5.52	105.34	111.36
1	C	895	VAL	N-CA-C	-5.51	105.16	110.72
1	B	813	TRP	N-CA-C	-5.49	104.70	111.40
1	D	594	ARG	N-CA-C	5.48	120.36	111.37
1	C	941	GLU	N-CA-C	5.43	117.27	108.26
1	C	815	LEU	N-CA-C	-5.39	105.30	111.07
1	D	800	ILE	N-CA-C	5.38	115.63	110.74
1	D	632	HIS	N-CA-C	5.36	116.36	107.73
1	D	821	GLU	N-CA-C	-5.25	105.20	111.03
1	D	641	LEU	N-CA-C	-5.25	104.48	112.04
1	D	649	SER	N-CA-C	-5.07	107.26	113.50
1	C	821	GLU	N-CA-C	-5.03	105.49	110.97
1	B	907	ASP	N-CA-C	-5.01	105.49	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2153	0	2160	148	0
1	B	2091	0	2104	157	0
1	C	2235	0	2259	165	0
1	D	2108	0	2122	155	0
2	A	3	0	0	0	0
2	B	6	0	0	1	0
2	C	5	0	0	0	0
All	All	8601	0	8645	604	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 35.

All (604) 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:D:924:THR:HG22	1:D:926:MET:H	1.09	1.14
1:B:769:ARG:HH11	1:B:769:ARG:HB3	1.22	1.00
1:B:769:ARG:HB3	1:B:769:ARG:NH1	1.78	0.97
1:D:858:LYS:H	1:D:858:LYS:HD2	1.34	0.92
1:C:657:ARG:HB2	1:C:789:GLU:HB2	1.52	0.92
1:C:593:LEU:HD23	1:C:664:GLU:HB3	1.48	0.92
1:C:940:ILE:HG13	1:C:959:ARG:HH22	1.36	0.91
1:C:976:LEU:HA	1:C:981:LEU:HD12	1.52	0.91
1:A:839:MET:HE3	1:A:839:MET:H	1.36	0.91
1:B:769:ARG:HG3	1:B:782:SER:HA	1.51	0.91
1:D:959:ARG:HD3	1:D:959:ARG:O	1.71	0.90
1:C:950:LYS:HE3	1:C:951:MET:HE3	1.54	0.89
1:A:806:ASN:HB2	1:A:919:ILE:O	1.73	0.89
1:B:909:TYR:HB2	1:B:969:ARG:HH11	1.41	0.85
1:A:885:ILE:HD11	1:A:888:ALA:HB3	1.58	0.85
1:B:983:VAL:O	1:B:984:LYS:HB2	1.76	0.84
1:A:932:LEU:HA	1:A:935:LEU:HD12	1.60	0.84
1:B:929:VAL:O	1:B:933:LYS:HB2	1.78	0.84
1:B:634:GLU:O	1:B:637:LEU:HB2	1.78	0.83
1:C:645:MET:HE3	1:D:641:LEU:HD22	1.60	0.83
1:B:805:LEU:HA	1:B:808:GLN:HE22	1.45	0.81
1:B:932:LEU:HA	1:B:935:LEU:HD12	1.62	0.81
1:B:798:ASP:O	1:B:802:SER:HB3	1.79	0.81
1:B:909:TYR:HB2	1:B:969:ARG:NH1	1.96	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:THR:O	1:B:781:LYS:HG2	1.80	0.80
1:A:940:ILE:HG21	1:A:959:ARG:NH2	1.96	0.80
1:D:893:THR:HG21	1:D:964:HIS:ND1	1.97	0.79
1:B:645:MET:HE2	1:B:645:MET:HA	1.64	0.78
1:B:894:GLU:OE2	1:B:966:PRO:HB3	1.84	0.77
1:A:652:HIS:CD2	1:A:653:GLN:H	2.02	0.77
1:C:976:LEU:HA	1:C:981:LEU:CD1	2.14	0.77
1:A:940:ILE:HG21	1:A:959:ARG:HH22	1.49	0.76
1:A:628:LYS:HD3	1:A:630:ILE:HD11	1.65	0.76
1:C:859:ASN:O	1:C:860:VAL:HG13	1.84	0.76
1:D:951:MET:HG3	1:D:954:GLU:HG3	1.67	0.76
1:B:845:GLU:CD	1:B:845:GLU:H	1.92	0.76
1:B:894:GLU:OE1	1:B:906:ILE:HG22	1.86	0.75
1:C:928:ARG:NH1	1:C:932:LEU:HD11	2.01	0.75
1:D:599:PHE:CE2	1:D:618:ASN:HB2	2.21	0.75
1:D:924:THR:HG22	1:D:926:MET:N	1.95	0.75
1:B:809:ARG:HA	1:B:812:TYR:CE2	2.22	0.75
1:D:847:ARG:HH11	1:D:847:ARG:HB3	1.51	0.74
1:B:958:ILE:O	1:B:962:ILE:HG12	1.87	0.74
1:D:858:LYS:HD2	1:D:858:LYS:N	2.03	0.73
1:C:806:ASN:CG	1:C:921:PRO:HB3	2.14	0.73
1:A:796:LEU:HD11	1:A:918:MET:HE3	1.71	0.72
1:A:910:SER:O	1:A:914:ILE:HG13	1.88	0.72
1:C:806:ASN:ND2	1:C:921:PRO:HB3	2.05	0.72
1:D:903:ASN:O	1:D:906:ILE:HG22	1.89	0.72
1:D:605:LEU:HD21	1:D:615:LYS:HB2	1.69	0.72
1:D:959:ARG:HD3	1:D:959:ARG:C	2.13	0.72
1:A:940:ILE:HG13	1:A:959:ARG:HH12	1.55	0.72
1:C:601:GLU:OE1	1:C:614:VAL:HG21	1.90	0.71
1:A:923:SER:HB3	1:A:927:GLU:OE2	1.91	0.71
1:B:769:ARG:HG3	1:B:782:SER:CA	2.20	0.71
1:C:922:PHE:CD2	1:C:928:ARG:HG3	2.26	0.71
1:A:657:ARG:HH22	1:B:594:ARG:HD2	1.55	0.71
1:D:893:THR:HG21	1:D:964:HIS:CE1	2.26	0.71
1:D:608:GLY:HA3	1:D:611:GLY:O	1.91	0.71
1:D:615:LYS:HG3	1:D:790:TYR:CE1	2.26	0.70
1:B:637:LEU:HD21	1:B:663:LEU:HD21	1.73	0.70
1:D:905:LYS:HE2	1:D:969:ARG:O	1.91	0.70
1:D:650:LEU:HD11	1:D:831:ILE:HD12	1.74	0.70
1:B:769:ARG:CG	1:B:782:SER:HA	2.22	0.70
1:B:799:LEU:HD11	1:B:843:ILE:HG13	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:GLU:OE2	1:B:969:ARG:NH2	2.26	0.69
1:C:946:PHE:CE2	1:C:955:LYS:HD2	2.27	0.69
1:A:926:MET:HA	1:A:929:VAL:HG23	1.75	0.69
1:C:806:ASN:HB2	1:C:921:PRO:HD3	1.74	0.68
1:C:953:VAL:C	1:C:955:LYS:H	2.02	0.68
1:D:840:ASN:HD22	1:D:853:ASP:HB2	1.59	0.68
1:C:799:LEU:HB3	1:C:805:LEU:HD22	1.74	0.68
1:A:805:LEU:HG	1:A:805:LEU:O	1.92	0.68
1:D:605:LEU:HD12	1:D:605:LEU:H	1.56	0.68
1:A:653:GLN:O	1:A:850:LYS:HE3	1.94	0.67
1:A:973:ARG:NH1	1:A:976:LEU:HD13	2.09	0.67
1:A:811:GLU:OE2	1:A:811:GLU:HA	1.95	0.67
1:C:771:PHE:CE2	1:D:830:GLY:HA3	2.30	0.67
1:B:940:ILE:HD13	1:B:959:ARG:NH1	2.10	0.67
1:C:959:ARG:O	1:C:959:ARG:HD3	1.94	0.67
1:B:796:LEU:HA	1:B:799:LEU:HD13	1.78	0.66
1:B:955:LYS:O	1:B:959:ARG:HB2	1.96	0.66
1:D:892:ALA:HA	1:D:909:TYR:CD2	2.30	0.66
1:C:985:HIS:HD2	1:C:986:GLN:H	1.43	0.66
1:B:903:ASN:O	1:B:906:ILE:HG23	1.96	0.66
1:C:923:SER:OG	1:C:924:THR:HG23	1.95	0.66
1:D:640:ILE:O	1:D:644:VAL:HG23	1.95	0.66
1:B:806:ASN:ND2	1:B:921:PRO:HB3	2.10	0.66
1:A:908:MET:HE2	1:A:972:ALA:N	2.11	0.66
1:A:942:PHE:HB3	1:A:943:PRO:HD2	1.78	0.66
1:B:616:ALA:HB3	1:B:627:ILE:HD13	1.78	0.65
1:B:805:LEU:HA	1:B:808:GLN:NE2	2.11	0.65
1:B:809:ARG:HA	1:B:812:TYR:CZ	2.32	0.65
1:B:769:ARG:HH11	1:B:769:ARG:CB	2.02	0.65
1:A:886:GLY:O	1:A:889:MET:HB2	1.97	0.65
1:B:652:HIS:HB2	1:B:825:TYR:CE2	2.31	0.65
1:B:640:ILE:O	1:B:644:VAL:HG23	1.96	0.65
1:A:971:GLY:O	1:A:974:THR:HB	1.97	0.65
1:C:784:LEU:HD11	1:D:645:MET:HE3	1.79	0.64
1:D:940:ILE:HD11	1:D:964:HIS:CD2	2.32	0.64
1:C:833:HIS:HD2	1:C:835:ASP:H	1.45	0.64
1:D:847:ARG:HB3	1:D:847:ARG:NH1	2.12	0.64
1:D:916:PHE:HB2	1:D:958:ILE:HD13	1.80	0.64
1:A:940:ILE:CG2	1:A:959:ARG:HH22	2.10	0.64
1:A:839:MET:H	1:A:839:MET:CE	2.10	0.63
1:C:768:ARG:O	1:C:769:ARG:HD2	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:LEU:C	1:B:639:THR:H	2.07	0.63
1:B:973:ARG:HE	1:B:973:ARG:HA	1.64	0.63
1:C:928:ARG:HH12	1:C:932:LEU:HD11	1.64	0.63
1:A:893:THR:HG21	1:A:964:HIS:CD2	2.34	0.63
1:A:795:THR:HG21	1:A:839:MET:O	1.99	0.63
1:C:812:TYR:CD1	1:C:812:TYR:C	2.77	0.63
1:D:610:PHE:HD2	1:D:610:PHE:N	1.96	0.63
1:D:903:ASN:O	1:D:905:LYS:N	2.32	0.62
1:B:896:LEU:O	1:B:897:ASP:C	2.41	0.62
1:C:613:VAL:CG2	1:C:628:LYS:HD2	2.30	0.62
1:D:815:LEU:HD22	1:D:849:VAL:HG12	1.81	0.62
1:A:795:THR:HB	1:A:838:PRO:O	1.99	0.62
1:B:961:LEU:O	1:B:969:ARG:HD3	1.99	0.62
1:A:896:LEU:O	1:A:897:ASP:HB2	1.99	0.62
1:C:816:PHE:CE2	1:C:820:LEU:HD11	2.34	0.62
1:B:664:GLU:O	1:B:782:SER:HB3	1.99	0.62
1:C:633:THR:OG1	1:C:636:LYS:HB2	1.99	0.62
1:A:943:PRO:HG2	1:A:946:PHE:HB2	1.81	0.61
1:B:641:LEU:O	1:B:645:MET:HG2	1.99	0.61
1:D:641:LEU:O	1:D:645:MET:HG2	2.00	0.61
1:D:947:ASP:CG	1:D:950:LYS:HB3	2.25	0.61
1:C:771:PHE:HE2	1:D:830:GLY:HA3	1.65	0.61
1:D:903:ASN:ND2	1:D:905:LYS:HB2	2.15	0.61
1:C:946:PHE:O	1:C:948:ASP:N	2.34	0.61
1:D:647:LEU:HD12	1:D:831:ILE:HD13	1.82	0.61
1:A:632:HIS:CD2	1:A:633:THR:H	2.19	0.61
1:A:641:LEU:HA	1:A:644:VAL:HG12	1.81	0.61
1:C:652:HIS:HD2	1:C:654:TYR:H	1.48	0.61
1:C:985:HIS:CD2	1:C:986:GLN:H	2.19	0.61
1:D:798:ASP:O	1:D:802:SER:HB2	2.00	0.61
1:B:919:ILE:HG13	1:B:920:TYR:N	2.16	0.61
1:C:812:TYR:C	1:C:812:TYR:HD1	2.09	0.61
1:C:851:ILE:N	1:C:851:ILE:HD12	2.16	0.61
1:B:804:ASN:HD22	1:B:807:GLN:HB2	1.66	0.61
1:C:652:HIS:CD2	1:C:654:TYR:H	2.19	0.61
1:D:844:ASP:C	1:D:846:SER:H	2.10	0.60
1:B:799:LEU:CD1	1:B:843:ILE:HG13	2.31	0.60
1:B:805:LEU:HD22	1:B:812:TYR:HB3	1.83	0.60
1:C:957:ILE:O	1:C:960:LEU:N	2.32	0.60
1:A:932:LEU:O	1:A:935:LEU:N	2.34	0.60
1:A:833:HIS:O	1:A:834:ARG:HB2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:MET:HE3	1:A:839:MET:N	2.13	0.60
1:D:613:VAL:HG22	1:D:628:LYS:HG3	1.83	0.60
1:B:634:GLU:O	1:B:637:LEU:CB	2.50	0.60
1:C:613:VAL:HG22	1:C:628:LYS:HD2	1.84	0.60
1:C:656:VAL:HG13	1:C:789:GLU:HB3	1.83	0.60
1:C:769:ARG:C	1:C:771:PHE:H	2.10	0.60
1:D:951:MET:HG3	1:D:954:GLU:CG	2.32	0.60
1:D:610:PHE:N	1:D:610:PHE:CD2	2.68	0.59
1:D:799:LEU:HA	1:D:803:GLU:HG3	1.84	0.59
1:A:892:ALA:HA	1:A:909:TYR:CD2	2.36	0.59
1:A:899:THR:HG22	1:A:899:THR:O	2.03	0.59
1:B:650:LEU:HD22	1:B:825:TYR:CE2	2.37	0.59
1:C:621:ASP:OD1	1:C:621:ASP:C	2.45	0.59
1:A:645:MET:SD	1:B:641:LEU:HD22	2.42	0.59
1:D:768:ARG:HG2	1:D:782:SER:OG	2.02	0.59
1:D:602:ILE:HG22	1:D:603:ALA:N	2.17	0.59
1:B:902:TYR:HB2	1:B:906:ILE:HG21	1.85	0.59
1:C:922:PHE:CE2	1:C:928:ARG:HG3	2.38	0.59
1:C:909:TYR:HA	1:C:961:LEU:O	2.03	0.59
1:C:796:LEU:O	1:C:800:ILE:HG13	2.02	0.58
1:B:633:THR:HB	1:B:637:LEU:HD13	1.85	0.58
1:C:950:LYS:CE	1:C:951:MET:HE3	2.29	0.58
1:C:615:LYS:HD3	1:C:790:TYR:CE1	2.37	0.58
1:C:634:GLU:HG3	1:C:782:SER:OG	2.02	0.58
1:B:784:LEU:HD23	1:B:784:LEU:C	2.28	0.58
1:B:981:LEU:N	1:B:981:LEU:HD12	2.19	0.58
1:A:641:LEU:O	1:A:645:MET:HG2	2.03	0.58
1:A:961:LEU:O	1:A:969:ARG:HD2	2.03	0.58
1:A:909:TYR:HA	1:A:961:LEU:O	2.04	0.57
1:C:632:HIS:CE1	1:C:636:LYS:HG2	2.39	0.57
1:C:931:ILE:HD12	1:C:943:PRO:HB3	1.86	0.57
1:C:957:ILE:O	1:C:960:LEU:HB2	2.04	0.57
1:D:631:ARG:HD2	1:D:783:THR:HG22	1.85	0.57
1:D:815:LEU:HD22	1:D:849:VAL:CG1	2.34	0.57
1:D:841:ILE:HG22	1:D:841:ILE:O	2.05	0.57
1:D:896:LEU:O	1:D:897:ASP:HB2	2.03	0.57
1:A:631:ARG:CB	1:A:783:THR:HG22	2.35	0.57
1:A:645:MET:HA	1:A:645:MET:HE2	1.87	0.57
1:D:823:LEU:O	1:D:826:ILE:N	2.37	0.57
1:B:845:GLU:CD	1:B:845:GLU:N	2.61	0.56
1:C:976:LEU:HD23	1:C:981:LEU:HD11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:840:ASN:HD22	1:D:853:ASP:CB	2.18	0.56
1:C:986:GLN:O	1:C:989:VAL:HB	2.05	0.56
1:D:658:TYR:CZ	1:D:788:MET:HE3	2.40	0.56
1:D:809:ARG:HA	1:D:812:TYR:CE2	2.39	0.56
1:B:889:MET:HG2	1:B:932:LEU:HD12	1.87	0.56
1:B:908:MET:O	1:B:961:LEU:HD22	2.05	0.56
1:C:908:MET:HE2	1:C:971:GLY:C	2.30	0.56
1:D:925:GLY:O	1:D:929:VAL:HG23	2.06	0.56
1:B:799:LEU:HD12	1:B:799:LEU:N	2.19	0.56
1:B:838:PRO:HD3	1:B:890:TYR:CE2	2.40	0.56
1:B:966:PRO:O	1:B:969:ARG:HB2	2.06	0.56
1:D:816:PHE:CE1	1:D:911:LEU:HD11	2.40	0.56
1:B:984:LYS:HA	1:B:984:LYS:NZ	2.21	0.56
1:C:769:ARG:C	1:C:771:PHE:N	2.64	0.56
1:D:894:GLU:OE1	1:D:966:PRO:HB3	2.06	0.56
1:A:621:ASP:OD2	1:A:623:ARG:HB2	2.06	0.55
1:C:985:HIS:CD2	1:C:986:GLN:N	2.74	0.55
1:D:618:ASN:HB3	1:D:621:ASP:OD1	2.07	0.55
1:D:983:VAL:O	1:D:984:LYS:CB	2.54	0.55
1:A:617:ARG:NH2	1:C:893:THR:HG22	2.21	0.55
1:C:617:ARG:HG3	1:C:617:ARG:HH11	1.71	0.55
1:C:932:LEU:O	1:C:935:LEU:N	2.36	0.55
1:D:820:LEU:HB2	1:D:976:LEU:HD21	1.88	0.55
1:D:594:ARG:O	1:D:598:ASP:HB2	2.07	0.55
1:D:903:ASN:HD21	1:D:905:LYS:HB2	1.72	0.55
1:A:645:MET:HB3	1:B:663:LEU:HB2	1.88	0.55
1:B:633:THR:O	1:B:781:LYS:CG	2.54	0.55
1:C:657:ARG:HB3	1:C:659:TYR:CE2	2.41	0.55
1:B:811:GLU:HA	1:B:811:GLU:OE2	2.07	0.55
1:C:657:ARG:HE	1:C:659:TYR:HE2	1.53	0.55
1:C:769:ARG:O	1:C:771:PHE:N	2.40	0.55
1:A:768:ARG:HD2	1:B:829:GLN:O	2.07	0.54
1:B:627:ILE:HD12	1:B:627:ILE:N	2.23	0.54
1:C:800:ILE:HG22	1:C:801:HIS:HD2	1.72	0.54
1:D:852:GLY:O	1:D:853:ASP:HB2	2.04	0.54
1:A:632:HIS:CD2	1:A:633:THR:HG23	2.42	0.54
1:A:839:MET:CE	1:A:839:MET:N	2.70	0.54
1:B:922:PHE:CE2	1:B:931:ILE:HD12	2.42	0.54
1:C:953:VAL:C	1:C:955:LYS:N	2.66	0.54
1:C:923:SER:HB3	1:C:927:GLU:HG3	1.90	0.54
1:A:808:GLN:O	1:A:811:GLU:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ILE:HG13	1:A:920:TYR:N	2.23	0.54
1:B:795:THR:HG23	1:B:798:ASP:OD1	2.08	0.54
1:B:805:LEU:CA	1:B:808:GLN:HE22	2.19	0.54
1:B:819:ILE:HG21	1:B:911:LEU:HD13	1.90	0.54
1:C:800:ILE:HG22	1:C:801:HIS:CD2	2.43	0.54
1:D:814:ARG:NH1	1:D:847:ARG:O	2.33	0.54
1:C:935:LEU:HD12	1:C:941:GLU:O	2.07	0.53
1:D:823:LEU:O	1:D:824:SER:C	2.50	0.53
1:C:965:ASP:C	1:C:967:ASN:H	2.16	0.53
1:B:769:ARG:CD	1:B:782:SER:HA	2.39	0.53
1:D:811:GLU:OE1	1:D:811:GLU:HA	2.07	0.53
1:B:800:ILE:HD13	1:B:917:GLU:HB3	1.90	0.53
1:D:983:VAL:O	1:D:984:LYS:HB3	2.09	0.53
1:A:632:HIS:HB3	1:A:637:LEU:HD13	1.91	0.53
1:C:946:PHE:CD2	1:C:955:LYS:HD2	2.44	0.53
1:D:947:ASP:C	1:D:949:ASN:H	2.16	0.53
1:D:612:GLN:HE21	1:D:614:VAL:CG1	2.21	0.53
1:A:933:LYS:NZ	1:A:933:LYS:HB2	2.23	0.53
1:A:934:LYS:HD2	1:A:941:GLU:OE1	2.09	0.53
1:B:769:ARG:HG3	1:B:782:SER:CB	2.39	0.53
1:D:605:LEU:H	1:D:605:LEU:CD1	2.17	0.53
1:D:804:ASN:HB3	1:D:807:GLN:NE2	2.23	0.53
1:D:983:VAL:O	1:D:984:LYS:HG2	2.09	0.52
1:A:817:ARG:NH1	1:A:981:LEU:HB3	2.23	0.52
1:A:885:ILE:HG12	1:A:886:GLY:N	2.24	0.52
1:C:640:ILE:O	1:C:644:VAL:HG23	2.08	0.52
1:A:909:TYR:CE2	1:A:913:ILE:HD11	2.45	0.52
1:A:653:GLN:HG3	1:A:654:TYR:CD2	2.45	0.52
1:B:647:LEU:HD21	1:B:854:PHE:CD2	2.44	0.52
1:B:835:ASP:OD2	1:B:837:LYS:HE2	2.09	0.52
1:D:804:ASN:HB3	1:D:807:GLN:CD	2.35	0.52
1:D:816:PHE:HE1	1:D:911:LEU:HD11	1.74	0.52
1:D:799:LEU:HD11	1:D:843:ILE:HG13	1.92	0.52
1:A:628:LYS:HD3	1:A:630:ILE:CD1	2.38	0.52
1:C:595:TYR:HE1	1:C:627:ILE:CD1	2.23	0.52
1:D:940:ILE:HD13	1:D:959:ARG:NH1	2.25	0.52
1:A:637:LEU:O	1:A:640:ILE:HG12	2.10	0.52
1:B:904:GLU:OE2	1:B:904:GLU:N	2.40	0.51
1:B:937:SER:C	1:B:939:SER:H	2.17	0.51
1:B:799:LEU:HD12	1:B:799:LEU:H	1.75	0.51
1:A:930:ASN:O	1:A:933:LYS:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:LYS:O	1:A:937:SER:HB3	2.11	0.51
1:A:922:PHE:CZ	1:A:932:LEU:HD11	2.45	0.51
1:A:978:SER:HG	1:A:980:TRP:CG	2.29	0.51
1:C:836:LEU:HB3	1:C:910:SER:OG	2.10	0.51
1:C:931:ILE:O	1:C:935:LEU:HD13	2.11	0.51
1:A:837:LYS:NZ	1:A:837:LYS:HB2	2.25	0.51
1:C:940:ILE:HG13	1:C:959:ARG:NH2	2.18	0.51
1:C:656:VAL:HG23	1:C:851:ILE:O	2.10	0.50
1:C:794:ARG:NH1	1:C:847:ARG:HH21	2.08	0.50
1:D:783:THR:OG1	1:D:785:PHE:CE1	2.62	0.50
1:A:628:LYS:CD	1:A:630:ILE:HD11	2.39	0.50
1:A:632:HIS:CD2	1:A:636:LYS:HG3	2.46	0.50
1:B:942:PHE:N	1:B:942:PHE:CD2	2.79	0.50
1:A:841:ILE:O	1:A:841:ILE:HG22	2.09	0.50
1:B:610:PHE:N	1:B:610:PHE:CD2	2.79	0.50
1:B:841:ILE:HG22	1:B:841:ILE:O	2.11	0.50
1:C:621:ASP:O	1:C:622:SER:HB2	2.10	0.50
1:D:605:LEU:CD1	1:D:613:VAL:HG12	2.41	0.50
1:D:894:GLU:OE1	1:D:969:ARG:NH2	2.45	0.50
1:B:942:PHE:N	1:B:942:PHE:HD2	2.09	0.50
1:A:942:PHE:N	1:A:942:PHE:CD1	2.79	0.50
1:B:632:HIS:O	1:B:632:HIS:CD2	2.64	0.50
1:A:634:GLU:HA	1:A:634:GLU:OE2	2.12	0.50
1:B:652:HIS:CD2	1:B:654:TYR:H	2.30	0.50
1:B:950:LYS:C	1:B:952:LYS:H	2.19	0.50
1:C:915:PHE:O	1:C:918:MET:HB2	2.11	0.50
1:D:799:LEU:HD22	1:D:847:ARG:NH2	2.27	0.50
1:B:612:GLN:O	1:B:629:LYS:HG2	2.11	0.50
1:B:621:ASP:C	1:B:623:ARG:H	2.20	0.50
1:B:804:ASN:O	1:B:808:GLN:NE2	2.44	0.50
1:A:812:TYR:CZ	1:A:919:ILE:HG22	2.47	0.49
1:B:837:LYS:H	1:B:840:ASN:HD21	1.60	0.49
1:B:937:SER:C	1:B:939:SER:N	2.70	0.49
1:C:820:LEU:HB2	1:C:976:LEU:HD21	1.92	0.49
1:A:942:PHE:HD1	1:A:942:PHE:H	1.60	0.49
1:B:954:GLU:O	1:B:958:ILE:HD12	2.12	0.49
1:D:769:ARG:O	1:D:770:ASN:C	2.55	0.49
1:B:923:SER:HB2	1:B:927:GLU:OE2	2.12	0.49
1:D:844:ASP:C	1:D:846:SER:N	2.68	0.49
1:D:858:LYS:H	1:D:858:LYS:CD	2.15	0.49
1:A:942:PHE:N	1:A:942:PHE:HD1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:ALA:HA	1:A:891:VAL:HG13	1.93	0.49
1:C:645:MET:CE	1:D:641:LEU:HD22	2.39	0.49
1:B:817:ARG:O	1:B:821:GLU:HG2	2.12	0.49
1:D:833:HIS:HD2	1:D:835:ASP:C	2.21	0.49
1:B:634:GLU:OE2	1:B:781:LYS:N	2.45	0.49
1:C:990:ILE:C	1:C:992:GLU:H	2.21	0.49
1:B:914:ILE:O	1:B:918:MET:HG3	2.12	0.48
1:B:973:ARG:HH11	1:B:976:LEU:CD1	2.26	0.48
1:B:645:MET:HA	1:B:645:MET:CE	2.41	0.48
1:C:655:VAL:HG22	1:C:826:ILE:HD11	1.96	0.48
1:C:953:VAL:HG13	1:C:954:GLU:N	2.28	0.48
1:A:619:ALA:CB	1:C:899:THR:HG21	2.43	0.48
1:A:908:MET:CE	1:A:972:ALA:N	2.76	0.48
1:C:607:GLN:OE1	1:C:612:GLN:HB3	2.13	0.48
1:D:638:SER:HA	1:D:641:LEU:HG	1.96	0.48
1:C:662:TRP:O	1:C:784:LEU:HD12	2.13	0.48
1:C:976:LEU:HD23	1:C:981:LEU:CD1	2.44	0.48
1:D:661:ALA:HA	1:D:785:PHE:O	2.13	0.48
1:C:618:ASN:HB3	1:C:621:ASP:OD2	2.14	0.48
1:D:903:ASN:O	1:D:906:ILE:CG2	2.60	0.48
1:A:607:GLN:HG3	1:A:612:GLN:HG2	1.95	0.48
1:B:822:ALA:O	1:B:826:ILE:HG13	2.14	0.48
1:C:611:GLY:HA3	1:C:629:LYS:O	2.13	0.48
1:C:892:ALA:HA	1:C:909:TYR:CD2	2.49	0.48
1:C:798:ASP:O	1:C:802:SER:N	2.46	0.48
1:A:926:MET:O	1:A:927:GLU:C	2.56	0.47
1:B:892:ALA:HB1	1:B:969:ARG:HH12	1.78	0.47
1:D:795:THR:OG1	1:D:797:TYR:HB3	2.13	0.47
1:A:838:PRO:HB2	1:A:839:MET:HE2	1.97	0.47
1:C:617:ARG:HH12	1:C:622:SER:C	2.23	0.47
1:B:916:PHE:CE2	1:B:935:LEU:HD11	2.50	0.47
1:A:631:ARG:HB2	1:A:783:THR:HG22	1.96	0.47
1:A:849:VAL:CG1	1:A:850:LYS:N	2.77	0.47
1:A:932:LEU:N	1:A:932:LEU:HD12	2.29	0.47
1:B:632:HIS:O	1:B:632:HIS:CG	2.67	0.47
1:D:932:LEU:O	1:D:936:ARG:HG2	2.13	0.47
1:D:947:ASP:O	1:D:949:ASN:N	2.47	0.47
1:A:940:ILE:CB	1:A:959:ARG:HH22	2.27	0.47
1:C:795:THR:HA	1:C:842:PHE:HA	1.96	0.47
1:D:631:ARG:O	1:D:632:HIS:HB2	2.14	0.47
1:D:956:LYS:NZ	1:D:980:TRP:CD2	2.83	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:HIS:HB2	1:D:825:TYR:CE2	2.50	0.47
1:B:637:LEU:O	1:B:639:THR:N	2.45	0.47
1:D:893:THR:O	1:D:895:VAL:N	2.48	0.47
1:A:849:VAL:HG12	1:A:850:LYS:N	2.30	0.47
1:C:641:LEU:HD22	1:D:645:MET:HE2	1.97	0.47
1:C:935:LEU:HD11	1:C:942:PHE:HA	1.97	0.47
1:D:598:ASP:CG	1:D:620:LEU:HD11	2.40	0.47
1:B:955:LYS:HA	1:B:958:ILE:HD12	1.97	0.47
1:C:650:LEU:CD2	1:C:829:GLN:HG3	2.45	0.47
1:C:817:ARG:O	1:C:821:GLU:HG2	2.15	0.47
1:D:924:THR:HG22	1:D:925:GLY:N	2.29	0.47
1:D:960:LEU:O	1:D:969:ARG:HG3	2.15	0.47
1:A:963:ASP:OD1	1:A:968:LYS:HB2	2.15	0.46
1:D:619:ALA:O	1:D:621:ASP:N	2.48	0.46
1:D:647:LEU:CD1	1:D:831:ILE:HD13	2.45	0.46
1:D:844:ASP:O	1:D:846:SER:N	2.47	0.46
1:D:890:TYR:O	1:D:910:SER:HB3	2.15	0.46
1:B:920:TYR:CE2	1:B:943:PRO:HG3	2.51	0.46
1:C:957:ILE:HA	1:C:960:LEU:HD12	1.97	0.46
1:D:621:ASP:O	1:D:622:SER:OG	2.26	0.46
1:A:951:MET:HB3	1:A:954:GLU:CG	2.45	0.46
1:B:819:ILE:CD1	1:B:841:ILE:HD13	2.45	0.46
1:B:821:GLU:O	1:B:824:SER:HB3	2.15	0.46
1:C:923:SER:OG	1:C:924:THR:N	2.45	0.46
1:C:957:ILE:O	1:C:958:ILE:C	2.58	0.46
1:A:603:ALA:O	1:A:614:VAL:HB	2.15	0.46
1:C:804:ASN:C	1:C:806:ASN:H	2.22	0.46
1:C:984:LYS:HE2	1:C:988:GLU:OE1	2.16	0.46
1:D:654:TYR:CD1	1:D:818:GLN:HB3	2.51	0.46
1:B:833:HIS:O	1:B:834:ARG:HB2	2.15	0.46
1:C:595:TYR:HE1	1:C:627:ILE:HD13	1.81	0.46
1:A:809:ARG:HA	1:A:812:TYR:CE2	2.51	0.46
1:A:959:ARG:HG2	1:A:959:ARG:HH21	1.80	0.46
1:B:932:LEU:O	1:B:936:ARG:HG3	2.16	0.46
1:B:942:PHE:CZ	1:B:959:ARG:HG2	2.51	0.46
1:A:930:ASN:O	1:A:931:ILE:C	2.57	0.46
1:A:959:ARG:NH2	1:A:959:ARG:HG2	2.31	0.46
1:C:621:ASP:OD1	1:C:623:ARG:N	2.49	0.46
1:A:788:MET:HE3	1:A:788:MET:HB2	1.84	0.46
1:C:804:ASN:N	1:C:804:ASN:ND2	2.62	0.46
1:D:947:ASP:C	1:D:949:ASN:N	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:ASP:O	1:A:802:SER:HB2	2.16	0.46
1:A:855:GLY:O	1:A:856:LEU:C	2.58	0.46
1:A:908:MET:HE2	1:A:971:GLY:C	2.41	0.46
1:B:637:LEU:C	1:B:639:THR:N	2.73	0.46
1:B:812:TYR:CD1	1:B:812:TYR:C	2.94	0.46
1:B:892:ALA:HB2	1:B:909:TYR:CB	2.46	0.46
1:D:613:VAL:CG2	1:D:628:LYS:HG3	2.46	0.46
1:D:633:THR:O	1:D:637:LEU:HG	2.16	0.46
1:D:946:PHE:CE2	1:D:951:MET:HB3	2.51	0.46
1:A:654:TYR:CB	1:A:822:ALA:HB2	2.46	0.45
1:A:794:ARG:HA	1:A:798:ASP:OD2	2.15	0.45
1:B:951:MET:HA	1:B:954:GLU:HG2	1.98	0.45
1:C:804:ASN:C	1:C:806:ASN:N	2.73	0.45
1:D:821:GLU:O	1:D:822:ALA:C	2.58	0.45
1:C:640:ILE:HA	1:C:643:GLU:OE1	2.17	0.45
1:C:798:ASP:O	1:C:799:LEU:C	2.60	0.45
1:B:858:LYS:HG2	1:B:902:TYR:OH	2.17	0.45
1:D:615:LYS:NZ	1:D:790:TYR:CZ	2.85	0.45
1:D:953:VAL:O	1:D:956:LYS:N	2.47	0.45
1:C:618:ASN:OD1	1:C:620:LEU:N	2.49	0.45
1:C:617:ARG:HG3	1:C:617:ARG:NH1	2.32	0.45
1:C:851:ILE:N	1:C:851:ILE:CD1	2.78	0.45
1:C:909:TYR:OH	1:C:936:ARG:HG2	2.16	0.45
1:A:645:MET:CB	1:B:663:LEU:HB2	2.47	0.45
1:A:805:LEU:O	1:A:812:TYR:HD2	2.00	0.45
1:B:621:ASP:O	1:B:623:ARG:N	2.50	0.45
1:B:652:HIS:HB2	1:B:825:TYR:CD2	2.52	0.45
1:C:845:GLU:C	1:C:847:ARG:H	2.25	0.45
1:C:953:VAL:O	1:C:955:LYS:N	2.49	0.45
1:D:828:SER:C	1:D:830:GLY:H	2.24	0.45
1:B:973:ARG:HE	1:B:973:ARG:CA	2.28	0.45
1:C:818:GLN:OE1	1:C:849:VAL:HG13	2.17	0.45
1:C:899:THR:C	1:C:901:HIS:H	2.23	0.45
1:B:935:LEU:C	1:B:937:SER:H	2.24	0.45
1:C:621:ASP:OD1	1:C:623:ARG:HG3	2.17	0.45
1:C:959:ARG:HD3	1:C:959:ARG:C	2.41	0.45
1:D:924:THR:CG2	1:D:925:GLY:N	2.80	0.45
1:A:654:TYR:HB3	1:A:822:ALA:HB2	1.98	0.44
1:D:599:PHE:CD2	1:D:618:ASN:HB2	2.51	0.44
1:A:835:ASP:O	1:A:840:ASN:ND2	2.51	0.44
1:B:825:TYR:O	1:B:828:SER:OG	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:929:VAL:O	1:B:929:VAL:HG12	2.17	0.44
1:B:621:ASP:C	1:B:623:ARG:N	2.75	0.44
1:B:812:TYR:CZ	1:B:919:ILE:HG22	2.53	0.44
1:B:813:TRP:HA	1:B:813:TRP:CE3	2.51	0.44
1:C:807:GLN:O	1:C:809:ARG:N	2.50	0.44
1:D:816:PHE:HE1	1:D:911:LEU:CD1	2.31	0.44
1:B:632:HIS:NE2	1:B:636:LYS:CE	2.80	0.44
1:B:637:LEU:HG	1:B:641:LEU:HG	1.98	0.44
1:C:621:ASP:OD1	1:C:623:ARG:CG	2.65	0.44
1:D:650:LEU:CD2	1:D:829:GLN:HG3	2.48	0.44
1:D:814:ARG:O	1:D:815:LEU:C	2.61	0.44
1:B:643:GLU:CD	1:B:834:ARG:HH22	2.25	0.44
1:C:615:LYS:HE2	1:C:624:TYR:CD2	2.52	0.44
1:C:784:LEU:CD1	1:D:645:MET:HE3	2.47	0.44
1:D:927:GLU:O	1:D:931:ILE:HG13	2.17	0.44
1:A:631:ARG:O	1:A:632:HIS:HB2	2.18	0.44
1:A:916:PHE:HB2	1:A:958:ILE:HD13	1.99	0.44
1:A:963:ASP:O	1:A:969:ARG:NH1	2.50	0.44
1:B:919:ILE:HG13	1:B:920:TYR:H	1.82	0.44
1:D:950:LYS:HE3	1:D:951:MET:SD	2.58	0.44
1:D:975:LEU:HD23	1:D:975:LEU:HA	1.89	0.44
1:A:600:GLU:HB2	1:C:898:GLY:O	2.17	0.44
1:A:812:TYR:CD1	1:A:812:TYR:C	2.95	0.44
1:B:891:VAL:O	1:B:892:ALA:C	2.59	0.44
1:D:770:ASN:HD22	1:D:770:ASN:N	2.16	0.44
1:D:893:THR:O	1:D:894:GLU:C	2.60	0.44
1:C:851:ILE:CD1	1:C:851:ILE:H	2.30	0.43
1:C:929:VAL:O	1:C:929:VAL:HG12	2.17	0.43
1:D:656:VAL:HG13	1:D:789:GLU:HB3	1.99	0.43
1:D:842:PHE:O	1:D:849:VAL:HA	2.18	0.43
1:B:886:GLY:HA2	1:B:889:MET:HE2	1.99	0.43
1:C:909:TYR:CD1	1:C:962:ILE:HA	2.53	0.43
1:C:965:ASP:O	1:C:967:ASN:N	2.51	0.43
1:A:652:HIS:CG	1:A:653:GLN:H	2.36	0.43
1:B:637:LEU:CD2	1:B:663:LEU:HD21	2.45	0.43
1:C:806:ASN:HA	1:C:918:MET:O	2.19	0.43
1:C:994:LEU:O	1:C:995:LYS:C	2.61	0.43
1:D:650:LEU:HD11	1:D:831:ILE:CD1	2.47	0.43
1:D:808:GLN:O	1:D:809:ARG:C	2.60	0.43
1:A:926:MET:C	1:A:928:ARG:N	2.74	0.43
1:C:933:LYS:HB2	1:C:933:LYS:NZ	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:833:HIS:CD2	1:D:835:ASP:C	2.97	0.43
1:B:806:ASN:HB2	1:B:919:ILE:O	2.18	0.43
1:C:647:LEU:HD11	1:C:854:PHE:CD2	2.54	0.43
1:A:617:ARG:HH22	1:C:893:THR:HG22	1.83	0.43
1:A:619:ALA:HB1	1:C:899:THR:HG21	2.00	0.43
1:A:944:PRO:HG2	1:A:945:ASP:OD1	2.18	0.43
1:B:809:ARG:NH1	1:B:954:GLU:OE2	2.52	0.43
1:B:909:TYR:HA	1:B:961:LEU:O	2.18	0.43
1:B:973:ARG:HB3	2:B:8:HOH:O	2.18	0.43
1:C:975:LEU:HD23	1:C:975:LEU:HA	1.77	0.43
1:D:896:LEU:O	1:D:897:ASP:CB	2.66	0.43
1:C:833:HIS:CD2	1:C:835:ASP:H	2.32	0.43
1:C:973:ARG:O	1:C:974:THR:C	2.60	0.43
1:A:944:PRO:HG2	1:A:945:ASP:H	1.83	0.43
1:C:836:LEU:HG	1:C:914:ILE:CD1	2.49	0.43
1:D:652:HIS:CE1	1:D:654:TYR:H	2.37	0.43
1:D:903:ASN:C	1:D:905:LYS:N	2.74	0.43
1:D:958:ILE:O	1:D:962:ILE:HG12	2.19	0.43
1:A:621:ASP:OD1	1:A:621:ASP:N	2.49	0.43
1:A:932:LEU:O	1:A:936:ARG:HG2	2.18	0.43
1:C:768:ARG:HH21	1:D:646:LEU:HD11	1.83	0.43
1:A:955:LYS:O	1:A:959:ARG:HB2	2.18	0.43
1:C:650:LEU:O	1:C:657:ARG:NH1	2.51	0.43
1:D:926:MET:N	1:D:926:MET:SD	2.92	0.43
1:A:833:HIS:HA	1:A:854:PHE:CD2	2.54	0.42
1:B:784:LEU:CD2	1:B:786:ILE:HG13	2.48	0.42
1:B:962:ILE:O	1:B:963:ASP:C	2.60	0.42
1:C:621:ASP:OD1	1:C:623:ARG:CB	2.67	0.42
1:D:631:ARG:HH12	1:D:769:ARG:HG3	1.83	0.42
1:D:885:ILE:HG23	1:D:885:ILE:O	2.18	0.42
1:A:613:VAL:HG22	1:A:628:LYS:HG2	2.01	0.42
1:A:928:ARG:O	1:A:929:VAL:C	2.62	0.42
1:A:947:ASP:OD2	1:A:947:ASP:C	2.61	0.42
1:B:922:PHE:CE2	1:B:928:ARG:HG3	2.54	0.42
1:C:595:TYR:CE1	1:C:627:ILE:HD13	2.54	0.42
1:C:833:HIS:O	1:C:834:ARG:HB2	2.19	0.42
1:D:631:ARG:HD2	1:D:783:THR:CG2	2.48	0.42
1:D:656:VAL:HG21	1:D:852:GLY:HA3	2.01	0.42
1:D:885:ILE:HD11	1:D:887:THR:HB	2.01	0.42
1:A:642:SER:O	1:A:646:LEU:HD12	2.18	0.42
1:A:808:GLN:O	1:A:809:ARG:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:GLU:CD	1:B:781:LYS:N	2.77	0.42
1:C:618:ASN:OD1	1:C:618:ASN:C	2.62	0.42
1:C:650:LEU:HD21	1:C:829:GLN:HG3	2.01	0.42
1:C:972:ALA:O	1:C:975:LEU:HB2	2.19	0.42
1:A:932:LEU:C	1:A:934:LYS:N	2.76	0.42
1:C:905:LYS:HG2	1:C:966:PRO:O	2.20	0.42
1:C:637:LEU:HD11	1:C:782:SER:O	2.19	0.42
1:D:887:THR:O	1:D:887:THR:HG22	2.19	0.42
1:A:947:ASP:OD1	1:A:950:LYS:HB2	2.20	0.42
1:C:646:LEU:HA	1:C:646:LEU:HD23	1.76	0.42
1:C:656:VAL:CG2	1:C:850:LYS:HG2	2.50	0.42
1:C:664:GLU:O	1:C:782:SER:HB2	2.20	0.42
1:C:928:ARG:NH1	1:C:932:LEU:CD1	2.77	0.42
1:A:613:VAL:HG22	1:A:628:LYS:CG	2.48	0.42
1:A:663:LEU:HB2	1:B:645:MET:HB3	2.01	0.42
1:B:653:GLN:HE21	1:B:653:GLN:HB3	1.55	0.42
1:C:771:PHE:HE2	1:D:830:GLY:CA	2.32	0.42
1:C:808:GLN:OE1	1:C:808:GLN:N	2.53	0.42
1:B:840:ASN:C	1:B:840:ASN:HD22	2.26	0.42
1:C:899:THR:HG22	1:C:900:GLY:H	1.85	0.42
1:D:819:ILE:HG21	1:D:911:LEU:HD21	2.01	0.42
1:A:610:PHE:CD1	1:A:610:PHE:N	2.88	0.42
1:D:768:ARG:HA	1:D:782:SER:CB	2.50	0.42
1:D:843:ILE:HA	1:D:848:ASN:O	2.20	0.42
1:A:926:MET:HA	1:A:929:VAL:CG2	2.46	0.41
1:C:804:ASN:O	1:C:808:GLN:OE1	2.38	0.41
1:D:929:VAL:O	1:D:933:LYS:HG2	2.20	0.41
1:A:645:MET:HG3	1:B:641:LEU:HD13	2.01	0.41
1:A:795:THR:HG21	1:A:839:MET:C	2.45	0.41
1:B:966:PRO:HA	1:B:969:ARG:HE	1.85	0.41
1:D:980:TRP:O	1:D:981:LEU:C	2.62	0.41
1:A:805:LEU:HA	1:A:805:LEU:HD12	1.80	0.41
1:B:784:LEU:C	1:B:784:LEU:CD2	2.92	0.41
1:C:610:PHE:HB3	1:C:631:ARG:O	2.20	0.41
1:D:605:LEU:HD13	1:D:613:VAL:HG12	2.02	0.41
1:A:640:ILE:HA	1:A:643:GLU:HG3	2.01	0.41
1:A:924:THR:OG1	1:A:927:GLU:HB2	2.21	0.41
1:B:812:TYR:HB2	1:B:918:MET:HE2	2.02	0.41
1:D:632:HIS:CE1	1:D:636:LYS:HD3	2.55	0.41
1:B:940:ILE:HD13	1:B:959:ARG:HH11	1.81	0.41
1:C:851:ILE:HD12	1:C:851:ILE:H	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:ASN:HD21	1:B:921:PRO:HB3	1.83	0.41
1:B:949:ASN:O	1:B:952:LYS:HB2	2.21	0.41
1:D:784:LEU:HD12	1:D:785:PHE:N	2.36	0.41
1:A:804:ASN:C	1:A:806:ASN:N	2.77	0.41
1:A:804:ASN:C	1:A:806:ASN:H	2.27	0.41
1:A:829:GLN:CA	1:A:829:GLN:NE2	2.84	0.41
1:A:890:TYR:O	1:A:910:SER:HB3	2.20	0.41
1:B:894:GLU:HG2	1:B:969:ARG:HH22	1.86	0.41
1:B:973:ARG:HH11	1:B:976:LEU:HD12	1.85	0.41
1:C:809:ARG:CZ	1:C:809:ARG:HB3	2.51	0.41
1:B:632:HIS:NE2	1:B:636:LYS:NZ	2.68	0.41
1:B:946:PHE:O	1:B:947:ASP:C	2.63	0.41
1:C:654:TYR:HD1	1:C:821:GLU:HB2	1.85	0.41
1:C:664:GLU:HG3	1:C:785:PHE:CE1	2.56	0.41
1:C:804:ASN:N	1:C:804:ASN:HD22	2.19	0.41
1:C:887:THR:O	1:C:887:THR:HG22	2.21	0.41
1:D:894:GLU:CD	1:D:969:ARG:HH22	2.29	0.41
1:A:656:VAL:HG23	1:A:851:ILE:O	2.21	0.41
1:C:806:ASN:OD1	1:C:807:GLN:HG3	2.21	0.41
1:D:621:ASP:OD2	1:D:623:ARG:HG3	2.21	0.41
1:D:846:SER:O	1:D:847:ARG:HB2	2.20	0.41
1:A:959:ARG:HH11	1:A:963:ASP:HA	1.85	0.40
1:A:960:LEU:HB3	1:A:970:PRO:HD3	2.02	0.40
1:A:964:HIS:O	1:A:966:PRO:HD3	2.21	0.40
1:C:915:PHE:O	1:C:916:PHE:C	2.63	0.40
1:D:854:PHE:O	1:D:856:LEU:HD12	2.22	0.40
1:D:903:ASN:O	1:D:904:GLU:C	2.62	0.40
1:A:647:LEU:HD13	1:A:831:ILE:HG21	2.03	0.40
1:A:835:ASP:CG	1:A:837:LYS:HE3	2.46	0.40
1:D:859:ASN:OD1	1:D:860:VAL:N	2.54	0.40
1:A:795:THR:C	1:A:797:TYR:H	2.29	0.40
1:A:902:TYR:CD1	1:A:902:TYR:C	2.98	0.40
1:A:976:LEU:HA	1:A:981:LEU:HD22	2.03	0.40
1:B:633:THR:HB	1:B:634:GLU:H	1.24	0.40
1:B:647:LEU:HD23	1:B:647:LEU:HA	1.95	0.40
1:B:654:TYR:O	1:B:850:LYS:HA	2.21	0.40
1:B:804:ASN:HB3	1:B:807:GLN:HB2	2.03	0.40
1:B:812:TYR:C	1:B:812:TYR:HD1	2.29	0.40
1:C:940:ILE:HG21	1:C:959:ARG:NH2	2.36	0.40
1:A:641:LEU:HA	1:A:644:VAL:CG1	2.49	0.40
1:D:813:TRP:O	1:D:816:PHE:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:TYR:HE1	1:A:789:GLU:HA	1.87	0.40
1:A:809:ARG:HA	1:A:812:TYR:CZ	2.56	0.40
1:A:820:LEU:HA	1:A:820:LEU:HD23	1.85	0.40
1:B:837:LYS:O	1:B:838:PRO:C	2.63	0.40
1:C:922:PHE:CG	1:C:928:ARG:HG3	2.57	0.40
1:D:931:ILE:O	1:D:935:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/303 (84%)	201 (79%)	42 (16%)	12 (5%)	2	11
1	B	246/303 (81%)	191 (78%)	46 (19%)	9 (4%)	2	15
1	C	265/303 (88%)	200 (76%)	51 (19%)	14 (5%)	1	9
1	D	250/303 (82%)	202 (81%)	34 (14%)	14 (6%)	1	8
All	All	1016/1212 (84%)	794 (78%)	173 (17%)	49 (5%)	2	11

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	858	LYS
1	C	770	ASN
1	D	904	GLU
1	A	639	THR
1	A	937	SER
1	A	947	ASP
1	B	622	SER
1	B	638	SER
1	C	594	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	808	GLN
1	C	947	ASP
1	C	948	ASP
1	D	620	LEU
1	D	894	GLU
1	D	895	VAL
1	D	948	ASP
1	A	802	SER
1	B	632	HIS
1	C	803	GLU
1	C	858	LYS
1	C	954	GLU
1	D	793	ASN
1	D	824	SER
1	D	845	GLU
1	D	897	ASP
1	A	636	LYS
1	A	897	ASP
1	A	905	LYS
1	A	929	VAL
1	B	804	ASN
1	B	897	ASP
1	C	622	SER
1	B	896	LEU
1	C	846	SER
1	C	966	PRO
1	C	994	LEU
1	D	802	SER
1	D	823	LEU
1	D	859	ASN
1	D	940	ILE
1	A	831	ILE
1	B	859	ASN
1	C	632	HIS
1	C	940	ILE
1	A	940	ILE
1	B	983	VAL
1	D	602	ILE
1	A	640	ILE
1	B	940	ILE

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	179/272 (66%)	164 (92%)	15 (8%)	10	37
1	B	227/272 (84%)	198 (87%)	29 (13%)	4	19
1	C	243/272 (89%)	216 (89%)	27 (11%)	6	25
1	D	229/272 (84%)	206 (90%)	23 (10%)	7	29
All	All	878/1088 (81%)	784 (89%)	94 (11%)	6	26

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	593	LEU
1	A	614	VAL
1	A	637	LEU
1	A	639	THR
1	A	810	ASP
1	A	812	TYR
1	A	829	GLN
1	A	837	LYS
1	A	839	MET
1	A	889	MET
1	A	897	ASP
1	A	933	LYS
1	A	942	PHE
1	A	959	ARG
1	A	981	LEU
1	B	593	LEU
1	B	598	ASP
1	B	601	GLU
1	B	605	LEU
1	B	617	ARG
1	B	633	THR
1	B	636	LYS
1	B	653	GLN
1	B	795	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	804	ASN
1	B	805	LEU
1	B	808	GLN
1	B	810	ASP
1	B	812	TYR
1	B	813	TRP
1	B	840	ASN
1	B	845	GLU
1	B	849	VAL
1	B	894	GLU
1	B	906	ILE
1	B	927	GLU
1	B	942	PHE
1	B	950	LYS
1	B	951	MET
1	B	954	GLU
1	B	959	ARG
1	B	973	ARG
1	B	981	LEU
1	B	984	LYS
1	C	593	LEU
1	C	614	VAL
1	C	617	ARG
1	C	621	ASP
1	C	622	SER
1	C	635	GLU
1	C	636	LYS
1	C	663	LEU
1	C	769	ARG
1	C	794	ARG
1	C	795	THR
1	C	803	GLU
1	C	812	TYR
1	C	813	TRP
1	C	838	PRO
1	C	841	ILE
1	C	849	VAL
1	C	851	ILE
1	C	859	ASN
1	C	860	VAL
1	C	896	LEU
1	C	911	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	923	SER
1	C	933	LYS
1	C	948	ASP
1	C	951	MET
1	C	956	LYS
1	D	605	LEU
1	D	610	PHE
1	D	615	LYS
1	D	639	THR
1	D	647	LEU
1	D	663	LEU
1	D	784	LEU
1	D	794	ARG
1	D	812	TYR
1	D	821	GLU
1	D	834	ARG
1	D	836	LEU
1	D	849	VAL
1	D	858	LYS
1	D	906	ILE
1	D	935	LEU
1	D	948	ASP
1	D	951	MET
1	D	953	VAL
1	D	954	GLU
1	D	959	ARG
1	D	969	ARG
1	D	984	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	GLN
1	A	612	GLN
1	A	652	HIS
1	A	829	GLN
1	A	967	ASN
1	B	607	GLN
1	B	612	GLN
1	B	652	HIS
1	B	653	GLN
1	B	787	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	793	ASN
1	B	804	ASN
1	B	807	GLN
1	B	808	GLN
1	B	840	ASN
1	B	964	HIS
1	B	967	ASN
1	C	652	HIS
1	C	770	ASN
1	C	801	HIS
1	C	804	ASN
1	C	833	HIS
1	C	859	ASN
1	C	930	ASN
1	C	985	HIS
1	D	607	GLN
1	D	612	GLN
1	D	770	ASN
1	D	787	GLN
1	D	806	ASN
1	D	833	HIS
1	D	840	ASN
1	D	930	ASN
1	D	967	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	261/303 (86%)	-0.32	1 (0%) 88 76	41, 71, 112, 125	2 (0%)
1	B	254/303 (83%)	-0.21	4 (1%) 70 47	40, 78, 116, 132	0
1	C	271/303 (89%)	-0.32	2 (0%) 84 66	41, 76, 110, 117	0
1	D	256/303 (84%)	-0.37	2 (0%) 82 64	37, 67, 106, 118	0
All	All	1042/1212 (85%)	-0.30	9 (0%) 81 61	37, 73, 111, 132	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	989	VAL	2.8
1	D	619	ALA	2.6
1	D	899	THR	2.4
1	C	772	VAL	2.3
1	C	770	ASN	2.3
1	B	632	HIS	2.2
1	B	886	GLY	2.2
1	B	895	VAL	2.2
1	B	610	PHE	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.