



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:56 AM UTC

PDB ID : 6F5P / pdb_00006f5p
Title : A mechanism for the activation of the influenza virus transcriptase
Authors : Serna Martin, I.; Grimes, J.M.
Deposited on : 2017-12-02
Resolution : 4.14 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:

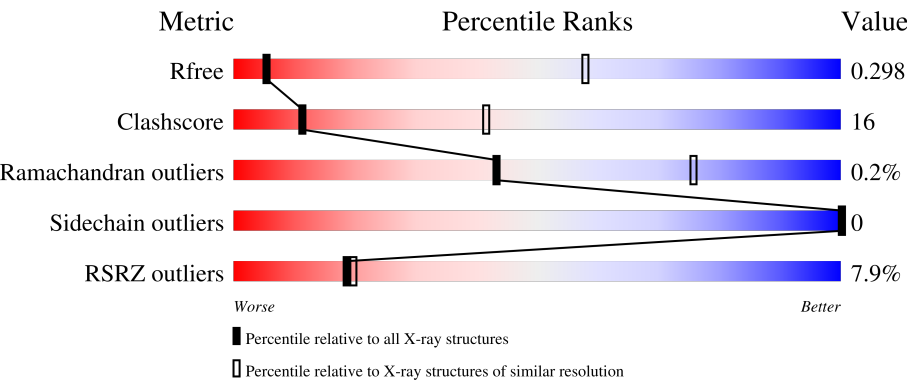
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.14 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.



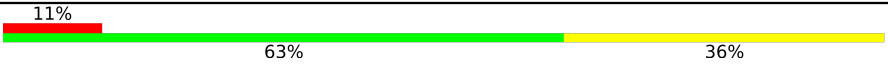
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1004 (4.46-3.82)
Clashscore	190562	1004 (4.44-3.84)
Ramachandran outliers	187476	1224 (4.48-3.80)
Sidechain outliers	187428	1211 (4.48-3.80)
RSRZ outliers	180081	1001 (4.46-3.82)

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	709	6% 64% 35% .
1	D	709	7% 66% 33% .
2	B	754	5% 66% 28% 6% .
2	C	754	5% 66% 29% .
3	E	774	13% 64% 35% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	774	
4	G	28	
5	H	10	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 35282 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5736	3654	972	1065	45			
1	D	708	Total	C	N	O	S	0	0	0
			5736	3654	972	1065	45			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	710	Total	C	N	O	S	0	0	0
			5643	3584	948	1057	54			
2	C	721	Total	C	N	O	S	0	0	0
			5736	3638	971	1073	54			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	771	Total	C	N	O	S	0	0	0
			6140	3883	1079	1141	37			
3	F	771	Total	C	N	O	S	0	0	0
			6140	3883	1079	1141	37			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	12	Total	C	N	O	P	0	0	0
			97	56	12	27	2			

- Molecule 5 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	10	Total	C	N	O	50	0	0
			50	30	10	10			

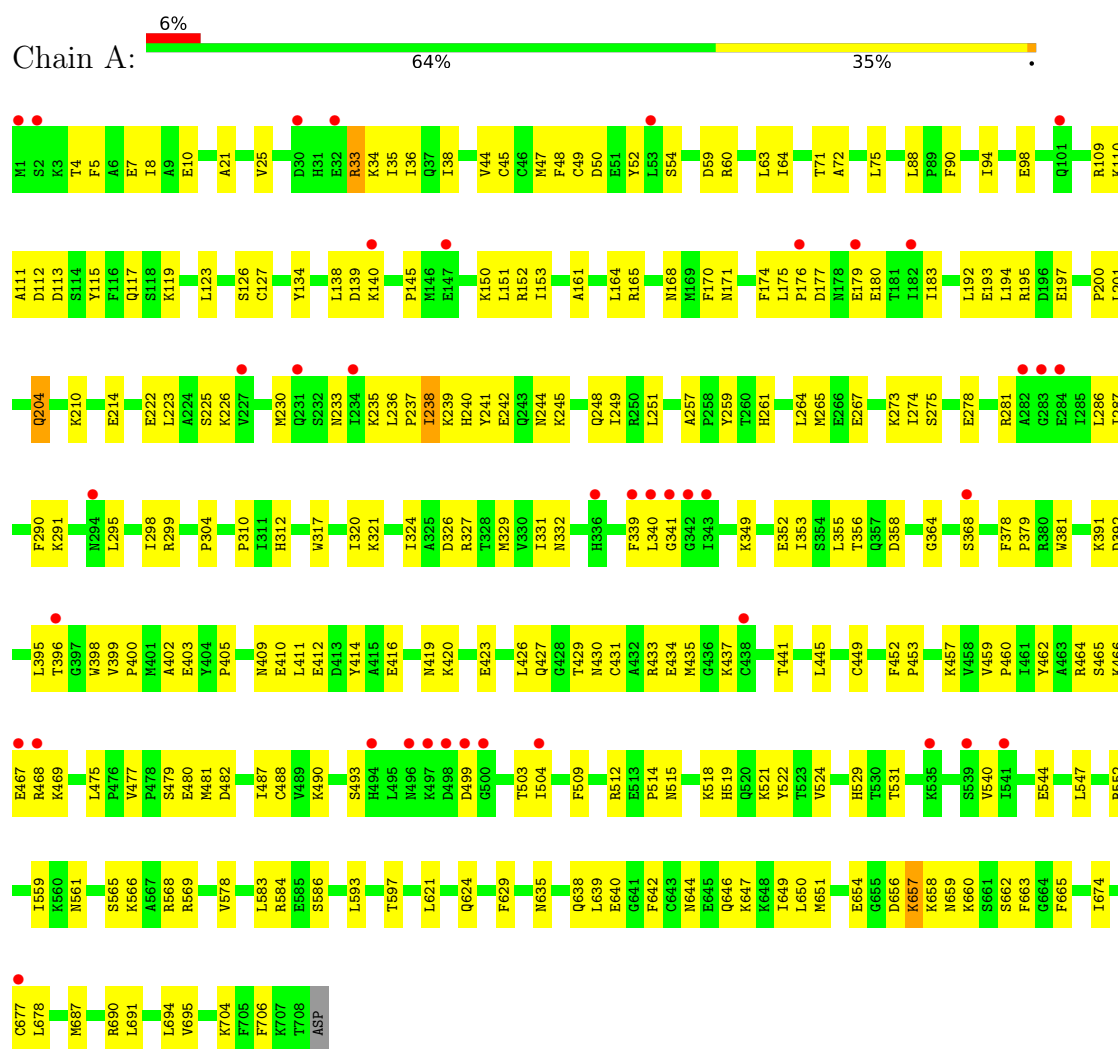
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Mg 2	0	0
6	D	2	Total 2	Mg 2	0	0

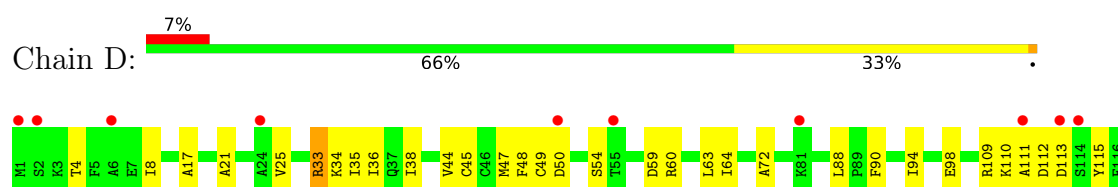
3 Residue-property plots

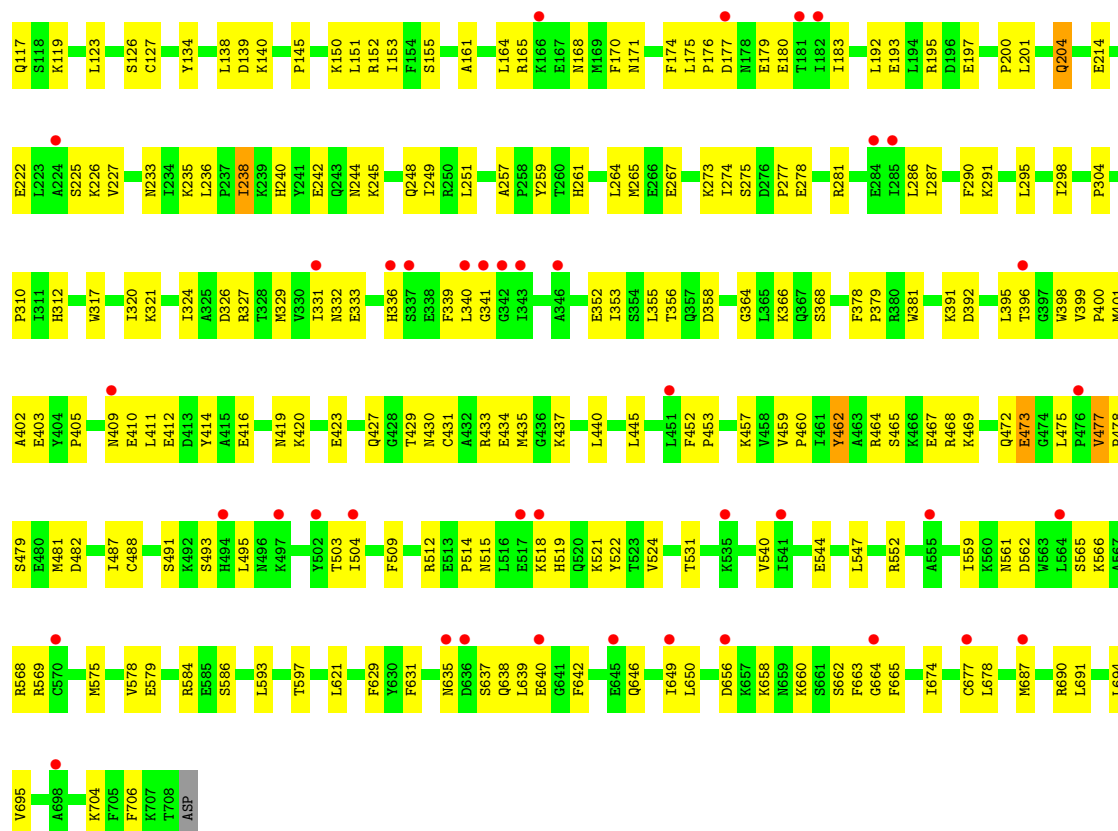
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polymerase acidic protein

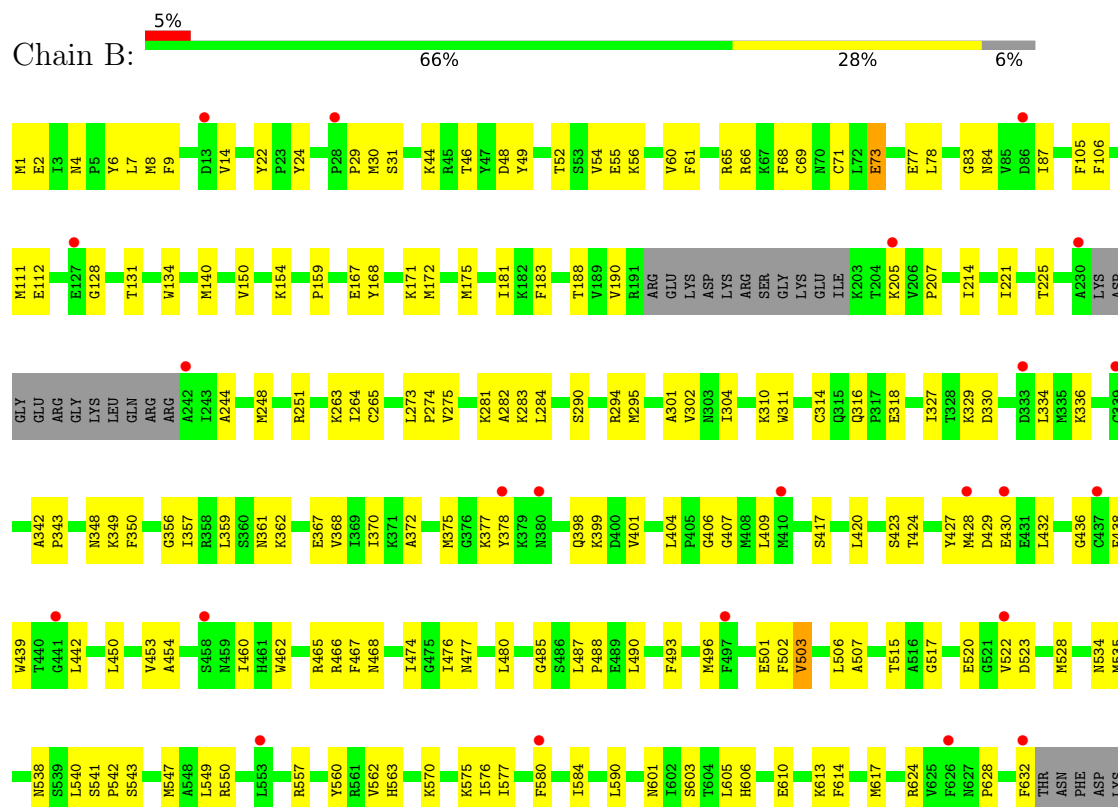


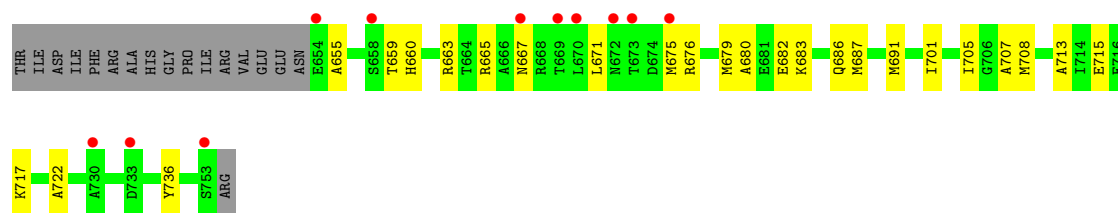
• Molecule 1: Polymerase acidic protein



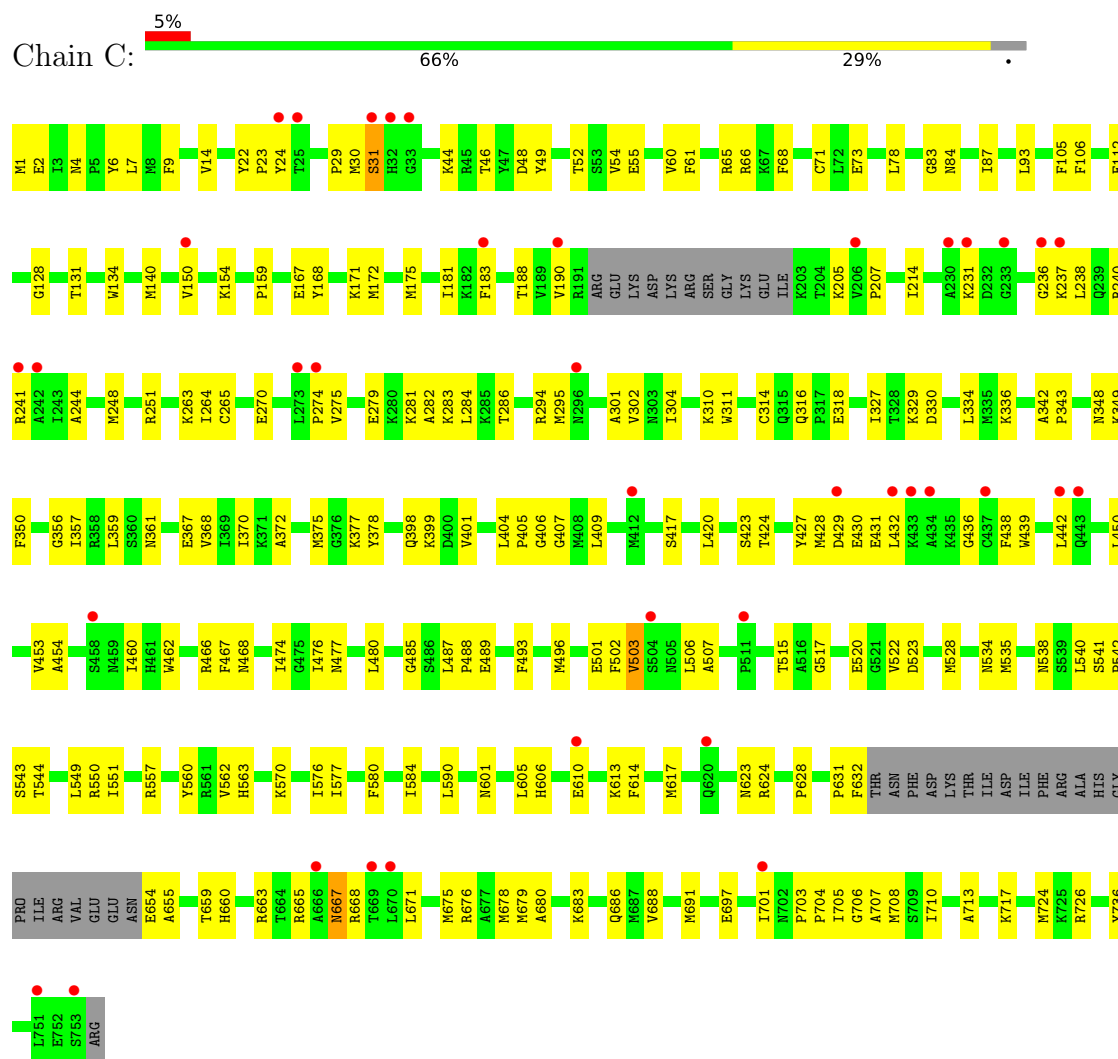


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

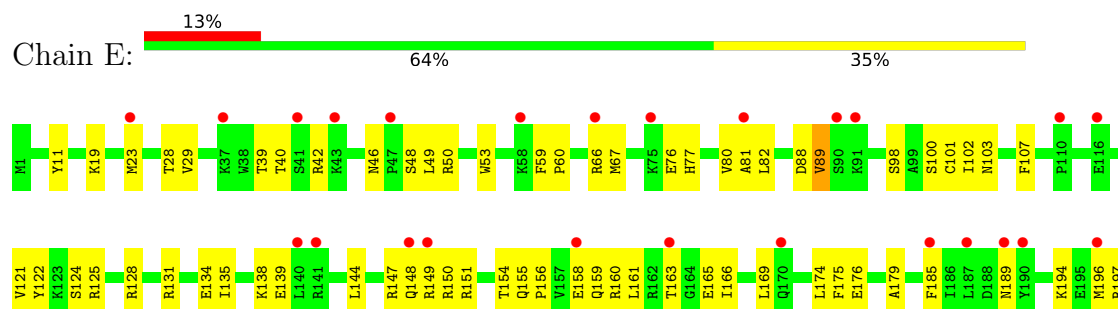


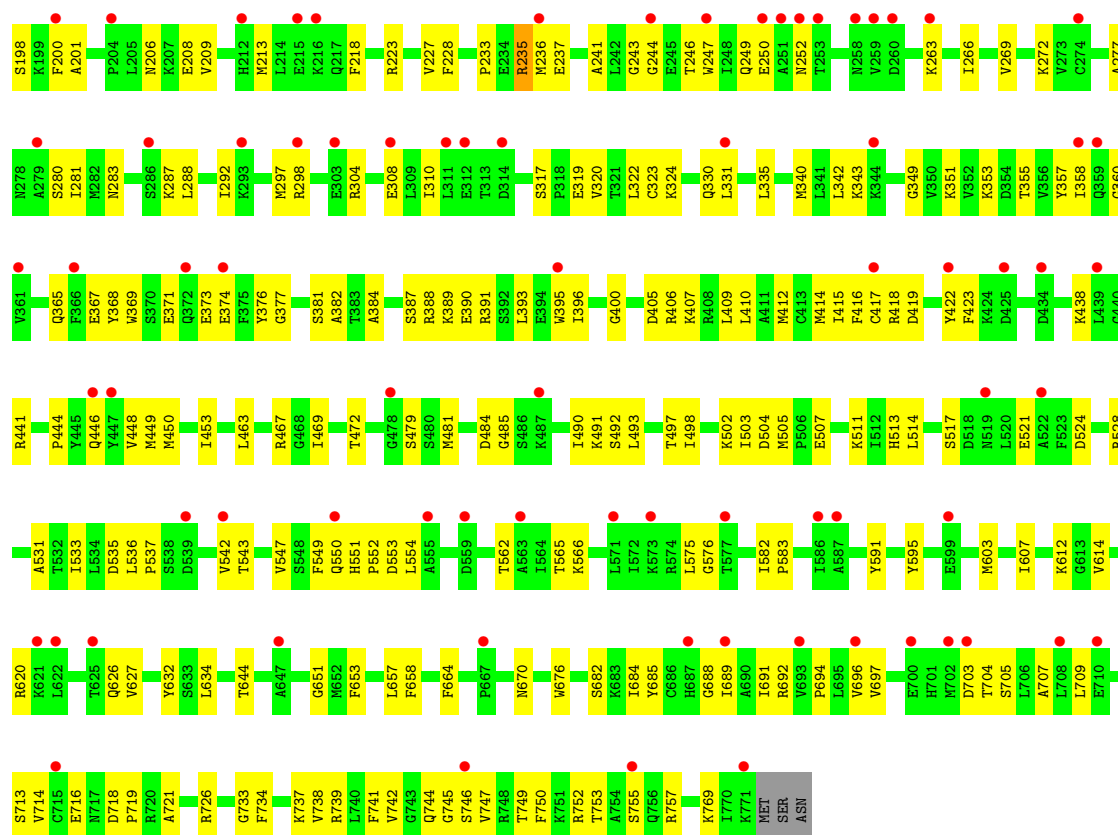


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

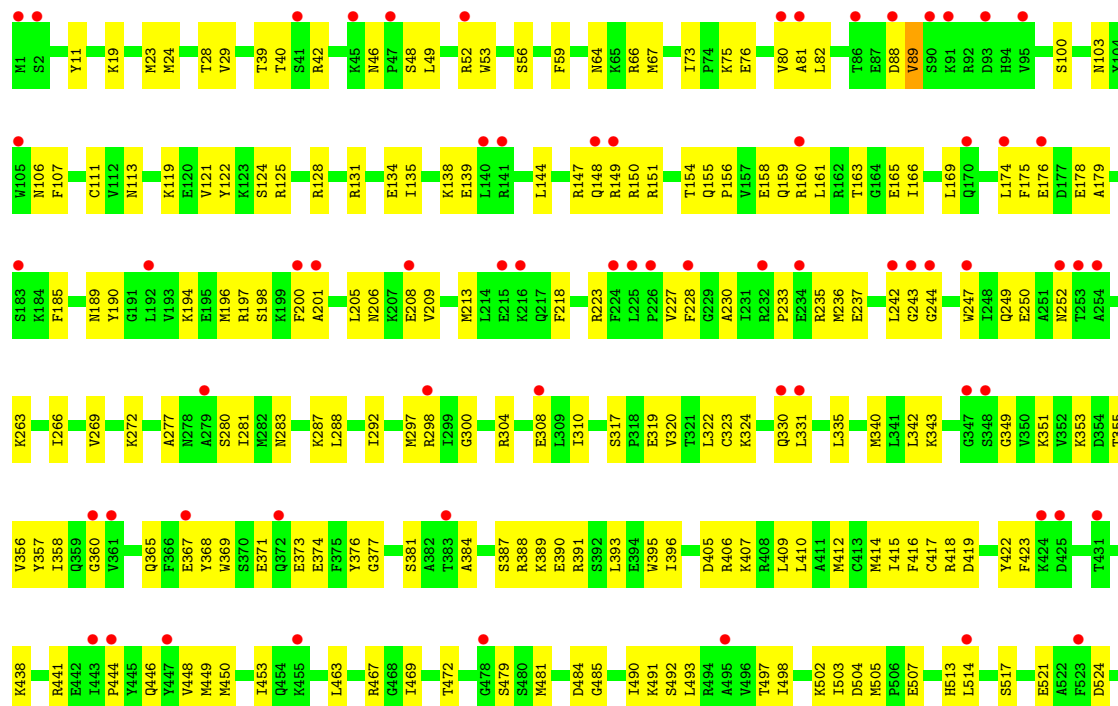


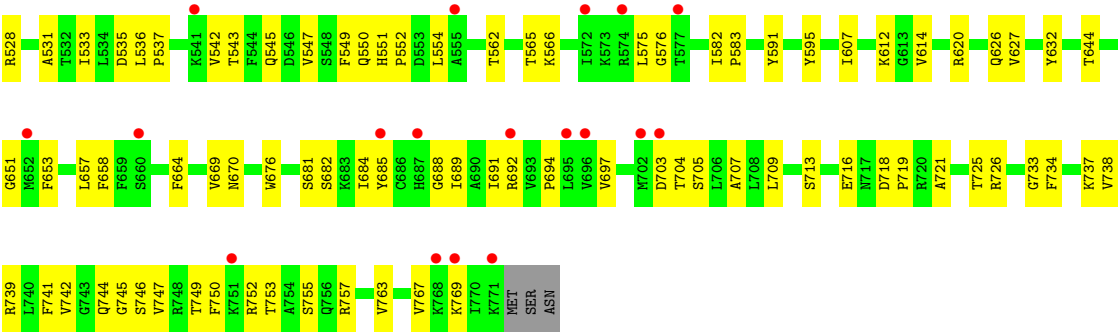
• Molecule 3: Polymerase basic protein 2



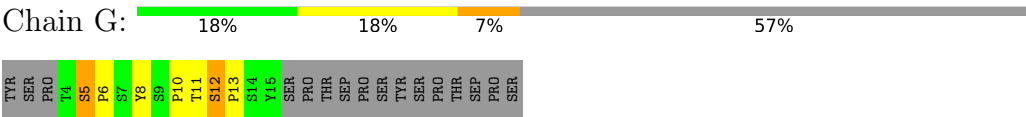


● Molecule 3: Polymerase basic protein 2





● Molecule 4: DNA-directed RNA polymerase subunit



● Molecule 5: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	185.70Å 185.70Å 597.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	131.31 – 4.14 131.31 – 4.14	Depositor EDS
% Data completeness (in resolution range)	68.9 (131.31-4.14) 68.9 (131.31-4.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 4.15Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.260 , 0.296 0.262 , 0.298	Depositor DCC
R_{free} test set	2819 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	105.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 145.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	35282	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: MG, SEP

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	0.24	1/5855 (0.0%)	0.54	12/7866 (0.2%)
1	D	0.24	2/5855 (0.0%)	0.54	9/7866 (0.1%)
2	B	0.20	0/5741	0.45	3/7716 (0.0%)
2	C	0.25	1/5835 (0.0%)	0.47	4/7839 (0.1%)
3	E	0.20	2/6251 (0.0%)	0.46	2/8415 (0.0%)
3	F	0.20	2/6251 (0.0%)	0.45	0/8415
4	G	0.30	0/79	0.60	0/105
5	H	0.54	0/49	2.90	8/67 (11.9%)
All	All	0.22	8/35916 (0.0%)	0.50	38/48289 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	4
2	B	0	1
2	C	0	1
All	All	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	30	MET	SD-CE	-8.09	1.59	1.79
3	F	249	GLN	CD-NE2	-7.50	1.17	1.33
3	E	249	GLN	CD-NE2	-7.42	1.17	1.33
1	A	238	ILE	CG1-CD1	-7.29	1.23	1.51
1	D	238	ILE	CG1-CD1	-7.16	1.23	1.51
3	E	249	GLN	CD-OE1	-6.25	1.11	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	249	GLN	CD-OE1	-6.15	1.11	1.23
1	D	462	TYR	CE1-CZ	-5.03	1.26	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	ALA	CB-CA-C	-10.83	95.31	111.77
5	H	7	ALA	N-CA-CB	-9.24	94.96	109.19
1	D	33	ARG	NE-CZ-NH2	9.08	127.37	119.20
5	H	3	ALA	N-CA-C	8.43	126.79	107.48
1	D	33	ARG	NE-CZ-NH1	-8.27	113.23	121.50
1	A	33	ARG	CD-NE-CZ	8.13	135.78	124.40
5	H	6	ALA	N-CA-C	7.96	121.53	108.08
1	A	512	ARG	NE-CZ-NH2	7.74	126.17	119.20
5	H	5	ALA	N-CA-C	7.64	119.25	111.07
1	D	33	ARG	CD-NE-CZ	7.63	135.08	124.40
5	H	7	ALA	N-CA-C	7.26	121.39	110.64
1	A	512	ARG	NE-CZ-NH1	-7.18	114.32	121.50
1	A	33	ARG	NE-CZ-NH2	-6.99	112.91	119.20
3	E	235	ARG	NE-CZ-NH2	6.94	125.44	119.20
2	C	30	MET	CG-SD-CE	6.69	115.63	100.90
2	C	31	SER	CA-CB-OG	6.50	124.10	111.10
2	C	1	MET	CB-CG-SD	6.48	132.14	112.70
2	B	1	MET	CB-CG-SD	6.45	132.04	112.70
1	A	177	ASP	N-CA-CB	-6.36	100.52	110.06
5	H	4	ALA	N-CA-C	6.07	120.76	112.68
1	A	657	LYS	CB-CG-CD	6.02	125.15	111.30
5	H	6	ALA	CB-CA-C	5.90	123.47	116.63
2	B	73	GLU	CA-CB-CG	5.88	125.85	114.10
1	A	512	ARG	CD-NE-CZ	5.84	132.57	124.40
3	E	235	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	A	340	LEU	CA-CB-CG	5.77	136.49	116.30
1	D	512	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	A	33	ARG	CG-CD-NE	-5.73	99.39	112.00
1	D	340	LEU	CA-CB-CG	5.61	135.92	116.30
1	A	657	LYS	CA-CB-CG	5.27	124.64	114.10
2	B	31	SER	CA-CB-OG	5.24	121.59	111.10
1	D	204	GLN	CA-CB-CG	-5.17	103.75	114.10
1	A	33	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	D	477	VAL	CA-CB-CG1	5.12	119.10	110.40
1	D	512	ARG	CD-NE-CZ	5.10	131.54	124.40
1	D	177	ASP	CA-CB-CG	5.09	117.69	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	667	ASN	CB-CG-ND2	-5.09	108.77	116.40
1	A	477	VAL	CG1-CB-CG2	-5.06	99.67	110.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	GLN	Sidechain
2	B	667	ASN	Sidechain
2	C	667	ASN	Sidechain
1	D	204	GLN	Sidechain
1	D	472	GLN	Peptide
1	D	473	GLU	Peptide
1	D	664	GLY	Peptide

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	5736	0	5749	235	0
1	D	5736	0	5749	224	0
2	B	5643	0	5736	195	0
2	C	5736	0	5837	214	0
3	E	6140	0	6250	220	0
3	F	6140	0	6250	236	0
4	G	97	0	73	11	0
5	H	50	0	52	0	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
All	All	35282	0	35696	1145	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 16.

All (1145) 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:410:GLU:OE1	1:D:411:LEU:N	1.59	1.34
1:A:410:GLU:OE1	1:A:411:LEU:N	1.59	1.34
3:E:367:GLU:O	3:E:418:ARG:NH1	1.87	1.08
3:F:367:GLU:O	3:F:418:ARG:NH1	1.87	1.07
1:A:410:GLU:OE1	1:A:411:LEU:HB2	1.57	1.05
1:D:410:GLU:OE1	1:D:411:LEU:HB2	1.57	1.04
1:A:410:GLU:OE1	1:A:411:LEU:CB	2.13	0.97
1:D:410:GLU:OE1	1:D:411:LEU:CB	2.13	0.96
1:A:690:ARG:HH12	2:B:2:GLU:HB3	1.30	0.93
3:E:228:PHE:HE2	3:E:235:ARG:HH11	0.91	0.91
1:D:233:ASN:HB2	2:C:78:LEU:HD12	1.52	0.91
3:F:228:PHE:HE2	3:F:235:ARG:NH1	1.68	0.90
1:A:410:GLU:CD	1:A:411:LEU:N	2.30	0.90
3:F:228:PHE:HE2	3:F:235:ARG:HH11	1.12	0.90
3:E:131:ARG:NH1	3:E:237:GLU:OE1	2.05	0.90
1:D:140:LYS:NZ	1:D:150:LYS:HE2	1.87	0.89
1:D:236:LEU:HD11	2:C:480:LEU:HD22	1.52	0.89
1:A:352:GLU:OE1	2:B:377:LYS:NZ	2.05	0.89
1:D:410:GLU:CD	1:D:411:LEU:N	2.30	0.89
2:C:665:ARG:HD2	3:F:89:VAL:HG21	1.53	0.89
1:D:410:GLU:OE1	1:D:411:LEU:CA	2.21	0.88
1:A:410:GLU:OE1	1:A:411:LEU:CA	2.21	0.88
1:A:140:LYS:NZ	1:A:150:LYS:HE2	1.87	0.88
3:F:131:ARG:NH1	3:F:237:GLU:OE1	2.05	0.88
2:C:65:ARG:HH21	2:C:348:ASN:HD21	1.23	0.86
1:D:304:PRO:HG3	1:D:310:PRO:HB3	1.57	0.86
1:A:204:GLN:HE22	2:B:56:LYS:HE3	1.38	0.86
3:E:228:PHE:HE2	3:E:235:ARG:NH1	1.74	0.86
1:A:304:PRO:HG3	1:A:310:PRO:HB3	1.56	0.85
2:C:496:MET:HA	2:C:503:VAL:HG21	1.60	0.84
2:B:496:MET:HA	2:B:503:VAL:HG21	1.60	0.84
2:B:65:ARG:HH21	2:B:348:ASN:HD21	1.23	0.83
1:D:690:ARG:HH12	2:C:2:GLU:HB3	1.44	0.83
2:B:686:GLN:OE1	3:E:39:THR:HG21	1.79	0.83
3:E:138:LYS:HB3	3:E:250:GLU:HG2	1.62	0.82
1:D:566:LYS:HE3	1:D:569:ARG:HH21	1.46	0.81
2:B:52:THR:HA	2:B:73:GLU:HG2	1.62	0.80
3:E:174:LEU:HD23	3:E:175:PHE:HB2	1.64	0.80
3:F:415:ILE:HD11	3:F:453:ILE:HD13	1.65	0.79
1:A:566:LYS:HE3	1:A:569:ARG:HH21	1.46	0.78
3:F:174:LEU:HD23	3:F:175:PHE:HB2	1.64	0.78
2:C:52:THR:HG22	2:C:54:VAL:H	1.48	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:THR:HG22	2:B:54:VAL:H	1.48	0.78
3:E:415:ILE:HD11	3:E:453:ILE:HD13	1.65	0.77
3:E:283:ASN:O	3:E:287:LYS:NZ	2.15	0.77
1:A:239:LYS:HZ1	4:G:6:PRO:HD2	1.48	0.77
1:D:235:LYS:HE2	1:D:235:LYS:HA	1.67	0.77
3:F:283:ASN:O	3:F:287:LYS:NZ	2.15	0.76
1:D:312:HIS:HB3	1:D:339:PHE:HZ	1.50	0.76
1:D:694:LEU:HD22	2:C:6:TYR:HB3	1.67	0.76
1:A:235:LYS:HA	1:A:235:LYS:HE2	1.68	0.76
1:A:312:HIS:HB3	1:A:339:PHE:HZ	1.50	0.76
1:A:257:ALA:HB3	1:A:379:PRO:HG3	1.68	0.76
1:D:257:ALA:HB3	1:D:379:PRO:HG3	1.68	0.75
3:E:547:VAL:HG13	3:E:688:GLY:HA2	1.67	0.75
3:F:547:VAL:HG13	3:F:688:GLY:HA2	1.66	0.75
1:A:171:ASN:ND2	2:B:167:GLU:OE2	2.19	0.75
1:A:419:ASN:ND2	2:B:543:SER:OG	2.19	0.75
1:D:640:GLU:OE2	2:C:29:PRO:HD3	1.87	0.75
1:A:151:LEU:HD13	3:E:753:THR:HG23	1.69	0.74
2:B:52:THR:CA	2:B:73:GLU:HG2	2.17	0.74
1:D:151:LEU:HD13	3:F:753:THR:HG23	1.69	0.74
3:F:272:LYS:HZ2	3:F:543:THR:HG23	1.53	0.74
3:E:272:LYS:HZ2	3:E:543:THR:HG23	1.49	0.73
3:F:298:ARG:NH1	3:F:684:ILE:HD11	2.03	0.73
1:A:238:ILE:HD13	1:A:663:PHE:HB2	1.69	0.73
3:F:128:ARG:NH1	3:F:155:GLN:HB3	2.03	0.73
3:E:128:ARG:NH1	3:E:155:GLN:HB3	2.02	0.73
3:F:670:ASN:HB3	3:F:676:TRP:H	1.53	0.73
1:D:658:LYS:HD3	1:D:660:LYS:HZ2	1.53	0.73
1:A:658:LYS:HD3	1:A:660:LYS:HZ2	1.54	0.73
1:A:240:HIS:NE2	1:A:656:ASP:OD2	2.21	0.73
3:E:298:ARG:NH1	3:E:684:ILE:HD11	2.03	0.73
3:E:235:ARG:HH21	3:E:252:ASN:HB2	1.52	0.73
1:A:140:LYS:HZ1	1:A:150:LYS:HE2	1.53	0.73
1:D:240:HIS:NE2	1:D:656:ASP:OD2	2.22	0.73
1:D:238:ILE:HD12	1:D:665:PHE:HA	1.72	0.72
3:E:670:ASN:HB3	3:E:676:TRP:H	1.53	0.72
3:E:575:LEU:HD13	3:E:582:ILE:HG13	1.71	0.72
2:C:576:ILE:HD11	3:F:100:SER:HB2	1.72	0.72
3:F:575:LEU:HD13	3:F:582:ILE:HG13	1.71	0.71
3:E:607:ILE:HB	3:E:612:LYS:HE3	1.72	0.71
1:A:237:PRO:HG3	4:G:5:SEP:O1P	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:HIS:HB3	1:D:339:PHE:CZ	2.25	0.71
2:C:679:MET:SD	3:F:42:ARG:NH2	2.64	0.71
2:C:154:LYS:HG2	2:C:159:PRO:HA	1.72	0.71
1:A:356:THR:HG22	2:B:377:LYS:NZ	2.05	0.71
1:D:368:SER:HB2	2:C:359:LEU:HD23	1.73	0.71
1:D:54:SER:OG	1:D:98:GLU:OE2	2.07	0.70
1:D:200:PRO:HG3	2:C:318:GLU:HB3	1.70	0.70
1:D:238:ILE:HD13	1:D:663:PHE:HB2	1.73	0.70
1:A:230:MET:HE1	2:B:465:ARG:HE	1.56	0.70
1:D:140:LYS:HZ1	1:D:150:LYS:HE2	1.52	0.70
3:F:418:ARG:NH2	3:F:446:GLN:OE1	2.24	0.70
3:E:324:LYS:NZ	3:E:331:LEU:HD22	2.07	0.70
1:D:226:LYS:NZ	2:C:431:GLU:HG3	2.07	0.70
1:D:469:LYS:HD3	1:D:475:LEU:HD13	1.74	0.70
1:A:312:HIS:HB3	1:A:339:PHE:CZ	2.26	0.70
2:B:131:THR:HG21	2:B:251:ARG:HD2	1.73	0.70
2:B:154:LYS:HG2	2:B:159:PRO:HA	1.73	0.70
3:F:607:ILE:HB	3:F:612:LYS:HE3	1.72	0.69
1:D:352:GLU:OE1	2:C:377:LYS:NZ	2.23	0.69
2:C:22:TYR:HD2	2:C:24:TYR:HE2	1.39	0.69
2:C:131:THR:HG21	2:C:251:ARG:HD2	1.73	0.69
2:C:190:VAL:HG22	2:C:205:LYS:HG2	1.75	0.69
1:A:694:LEU:HD22	2:B:6:TYR:HB3	1.74	0.69
3:F:324:LYS:NZ	3:F:331:LEU:HD22	2.07	0.69
3:E:160:ARG:HE	3:E:263:LYS:NZ	1.91	0.69
1:D:412:GLU:HG2	2:C:601:ASN:ND2	2.07	0.69
2:B:190:VAL:HG22	2:B:205:LYS:HG2	1.75	0.69
2:B:275:VAL:HG21	2:B:283:LYS:NZ	2.07	0.69
3:E:197:ARG:HD3	3:E:704:THR:HG22	1.74	0.69
2:B:701:ILE:HD11	3:E:208:GLU:HA	1.74	0.68
2:C:275:VAL:HG21	2:C:283:LYS:NZ	2.07	0.68
1:A:659:ASN:ND2	4:G:12:SEP:O	2.25	0.68
1:D:49:CYS:SG	1:D:50:ASP:N	2.66	0.68
2:C:282:ALA:HB3	3:F:149:ARG:HD3	1.76	0.68
3:F:160:ARG:H	3:F:160:ARG:HD3	1.59	0.68
3:F:197:ARG:HD3	3:F:704:THR:HG22	1.74	0.68
1:A:21:ALA:HA	1:A:38:ILE:HD11	1.76	0.68
1:A:464:ARG:HG2	1:A:482:ASP:HB3	1.74	0.68
3:F:160:ARG:HE	3:F:263:LYS:NZ	1.91	0.68
2:B:517:GLY:N	2:B:523:ASP:OD1	2.27	0.68
1:D:21:ALA:HA	1:D:38:ILE:HD11	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:682:GLU:OE1	3:E:42:ARG:NH2	2.27	0.68
2:B:22:TYR:HD2	2:B:24:TYR:HE2	1.40	0.68
1:A:138:LEU:HD11	1:A:140:LYS:HE3	1.76	0.68
1:A:200:PRO:HB3	2:B:69:CYS:HB2	1.76	0.67
1:D:414:TYR:HE2	2:C:542:PRO:HG2	1.58	0.67
1:A:238:ILE:HD12	1:A:665:PHE:HA	1.75	0.67
3:E:319:GLU:HG3	3:E:535:ASP:OD2	1.95	0.67
3:E:419:ASP:OD2	3:E:467:ARG:NH1	2.27	0.67
4:G:11:THR:OG1	4:G:12:SEP:O1P	2.10	0.67
1:A:331:ILE:O	1:A:332:ASN:ND2	2.28	0.67
3:F:310:ILE:HD13	3:F:323:CYS:HB3	1.75	0.67
1:A:690:ARG:NH2	2:B:2:GLU:OE1	2.25	0.67
1:D:45:CYS:O	1:D:48:PHE:HB3	1.94	0.67
3:F:319:GLU:HG3	3:F:535:ASP:OD2	1.95	0.67
1:A:356:THR:HG22	2:B:377:LYS:HZ1	1.59	0.67
3:E:418:ARG:NH2	3:E:446:GLN:OE1	2.25	0.66
2:C:517:GLY:N	2:C:523:ASP:OD1	2.27	0.66
3:F:384:ALA:HA	3:F:503:ILE:HD12	1.77	0.66
1:D:399:VAL:HB	1:D:427:GLN:HE22	1.61	0.66
2:B:675:MET:O	2:B:679:MET:HG2	1.95	0.66
3:E:310:ILE:HD13	3:E:323:CYS:HB3	1.75	0.66
3:F:419:ASP:OD2	3:F:467:ARG:NH1	2.28	0.66
1:A:54:SER:HB2	1:A:60:ARG:HE	1.60	0.66
1:D:138:LEU:HD11	1:D:140:LYS:HE3	1.76	0.66
1:D:464:ARG:HG2	1:D:482:ASP:HB3	1.75	0.66
1:A:204:GLN:NE2	2:B:56:LYS:HE3	2.11	0.66
2:C:350:PHE:HB3	2:C:401:VAL:HG21	1.78	0.66
1:A:44:VAL:HG13	1:A:153:ILE:HD11	1.77	0.66
1:D:44:VAL:HG13	1:D:153:ILE:HD11	1.77	0.66
1:D:575:MET:HG2	2:C:544:THR:HA	1.77	0.66
1:A:236:LEU:HD11	2:B:480:LEU:HD22	1.77	0.66
3:E:160:ARG:HD3	3:E:160:ARG:H	1.59	0.66
1:A:469:LYS:HD3	1:A:475:LEU:HD13	1.76	0.65
3:F:737:LYS:HA	3:F:750:PHE:O	1.96	0.65
2:C:675:MET:O	2:C:679:MET:HG2	1.95	0.65
3:E:737:LYS:HA	3:E:750:PHE:O	1.96	0.65
1:D:265:MET:HG2	1:D:434:GLU:HG2	1.79	0.65
3:E:384:ALA:HA	3:E:503:ILE:HD12	1.77	0.65
1:A:59:ASP:OD2	3:E:769:LYS:NZ	2.28	0.65
1:D:331:ILE:O	1:D:332:ASN:ND2	2.28	0.65
3:F:160:ARG:HE	3:F:263:LYS:HZ2	1.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASP:HB2	1:A:139:ASP:HB2	1.79	0.65
1:A:561:ASN:O	1:A:565:SER:HB3	1.97	0.65
3:F:272:LYS:NZ	3:F:543:THR:HG23	2.12	0.65
1:A:399:VAL:HB	1:A:427:GLN:HE22	1.61	0.65
1:D:658:LYS:HD3	1:D:660:LYS:NZ	2.11	0.65
2:B:350:PHE:HB3	2:B:401:VAL:HG21	1.78	0.64
3:E:272:LYS:NZ	3:E:543:THR:HG23	2.12	0.64
1:D:561:ASN:O	1:D:565:SER:HB3	1.97	0.64
2:B:683:LYS:HA	2:B:686:GLN:HG2	1.79	0.64
3:E:358:ILE:HG13	3:E:360:GLY:H	1.63	0.64
1:A:134:TYR:HB3	1:A:161:ALA:HB2	1.80	0.64
1:D:112:ASP:HB2	1:D:139:ASP:HB2	1.79	0.64
3:E:355:THR:HG22	3:E:365:GLN:HG2	1.80	0.64
2:B:432:LEU:HD23	2:B:466:ARG:HH12	1.62	0.64
3:E:551:HIS:O	3:E:551:HIS:ND1	2.30	0.64
1:A:265:MET:HG2	1:A:434:GLU:HG2	1.79	0.64
1:D:49:CYS:SG	1:D:63:LEU:HD11	2.38	0.64
2:B:398:GLN:HG3	2:B:399:LYS:H	1.63	0.64
2:B:679:MET:SD	3:E:42:ARG:NH2	2.70	0.64
1:A:531:THR:HG22	1:A:544:GLU:HG2	1.80	0.64
3:E:138:LYS:HB3	3:E:250:GLU:CG	2.28	0.63
3:F:280:SER:HB3	3:F:287:LYS:HE2	1.79	0.63
1:A:299:ARG:HE	3:F:545:GLN:HE22	1.46	0.63
1:D:134:TYR:HB3	1:D:161:ALA:HB2	1.80	0.63
2:C:172:MET:HA	2:C:175:MET:HE2	1.80	0.63
1:D:531:THR:HG22	1:D:544:GLU:HG2	1.80	0.63
2:C:349:LYS:NZ	2:C:407:GLY:O	2.32	0.63
2:C:398:GLN:HG3	2:C:399:LYS:H	1.63	0.63
3:F:551:HIS:O	3:F:551:HIS:ND1	2.30	0.63
2:C:237:LYS:HE2	2:C:241:ARG:HE	1.62	0.63
1:A:201:LEU:HD21	2:B:87:ILE:HD11	1.81	0.62
1:A:658:LYS:HD3	1:A:660:LYS:NZ	2.12	0.62
2:C:624:ARG:HA	3:F:111:CYS:HB2	1.81	0.62
3:E:280:SER:HB3	3:E:287:LYS:HE2	1.80	0.62
1:A:584:ARG:NH1	2:B:501:GLU:HG2	2.13	0.62
3:F:156:PRO:HG3	3:F:233:PRO:HB2	1.81	0.62
3:F:235:ARG:HH21	3:F:252:ASN:HB2	1.63	0.62
1:D:320:ILE:HG21	1:D:487:ILE:HG21	1.82	0.62
3:F:415:ILE:HG21	3:F:450:MET:HG2	1.81	0.62
3:F:358:ILE:HG13	3:F:360:GLY:H	1.63	0.62
1:A:49:CYS:SG	1:A:63:LEU:HD11	2.39	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:OE2	1:A:437:LYS:HD3	1.99	0.62
2:C:701:ILE:HD11	3:F:208:GLU:HA	1.81	0.62
1:A:320:ILE:HG21	1:A:487:ILE:HG21	1.82	0.62
1:A:244:ASN:HB2	1:A:704:LYS:O	2.00	0.62
1:A:521:LYS:HD2	1:A:552:ARG:NH1	2.15	0.62
3:E:156:PRO:HG3	3:E:233:PRO:HB2	1.81	0.62
3:F:355:THR:HG22	3:F:365:GLN:HG2	1.80	0.62
1:D:434:GLU:OE2	1:D:437:LYS:HD3	2.00	0.61
1:D:521:LYS:HD2	1:D:552:ARG:NH1	2.15	0.61
2:B:172:MET:HA	2:B:175:MET:HE2	1.81	0.61
2:B:349:LYS:NZ	2:B:407:GLY:O	2.32	0.61
3:F:536:LEU:HD12	3:F:537:PRO:HD2	1.83	0.61
1:D:341:GLY:H	1:D:503:THR:HG21	1.65	0.61
3:E:159:GLN:HA	3:E:304:ARG:HH12	1.66	0.61
2:B:282:ALA:HB3	3:E:149:ARG:HD3	1.82	0.61
2:C:432:LEU:HD23	2:C:466:ARG:HH12	1.63	0.61
1:D:244:ASN:HB2	1:D:704:LYS:O	2.00	0.61
3:E:298:ARG:HH12	3:E:684:ILE:HD11	1.64	0.61
3:F:298:ARG:HH12	3:F:684:ILE:HD11	1.65	0.61
1:A:183:ILE:HD13	2:B:334:LEU:HD22	1.83	0.61
3:E:415:ILE:HG21	3:E:450:MET:HG2	1.81	0.61
1:D:259:TYR:HE1	1:D:261:HIS:HB3	1.66	0.61
2:C:624:ARG:NH1	3:F:107:PHE:O	2.31	0.61
3:E:159:GLN:HA	3:E:304:ARG:NH1	2.16	0.61
3:F:159:GLN:HA	3:F:304:ARG:HH12	1.66	0.61
3:F:576:GLY:HA2	3:F:583:PRO:HG3	1.83	0.61
1:A:222:GLU:HA	1:A:225:SER:HB3	1.82	0.61
1:A:259:TYR:HE1	1:A:261:HIS:HB3	1.66	0.61
2:B:584:ILE:HG21	2:B:590:LEU:HD21	1.83	0.61
3:E:536:LEU:HD12	3:E:537:PRO:HD2	1.83	0.61
2:C:31:SER:HB3	2:C:240:ARG:HD2	1.83	0.61
2:C:372:ALA:HA	2:C:375:MET:HE2	1.83	0.61
2:C:683:LYS:HA	2:C:686:GLN:HG2	1.83	0.61
3:E:66:ARG:HE	3:E:67:MET:HE2	1.66	0.61
3:E:576:GLY:HA2	3:E:583:PRO:HG3	1.83	0.61
1:D:222:GLU:HA	1:D:225:SER:HB3	1.83	0.60
1:A:240:HIS:HB2	1:A:662:SER:O	2.01	0.60
2:B:632:PHE:CD1	3:E:102:ILE:HG12	2.36	0.60
3:F:159:GLN:HA	3:F:304:ARG:NH1	2.16	0.60
1:D:17:ALA:HB2	3:F:763:VAL:HG11	1.83	0.60
1:A:391:LYS:O	1:A:430:ASN:ND2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:MET:HG3	3:F:725:THR:HG21	1.84	0.60
3:E:138:LYS:HD3	3:E:250:GLU:HG2	1.84	0.60
3:E:281:ILE:HD11	3:E:438:LYS:HB2	1.84	0.60
1:D:240:HIS:HB2	1:D:662:SER:O	2.00	0.60
1:D:578:VAL:HG21	1:D:621:LEU:HG	1.83	0.60
1:D:329:MET:SD	1:D:329:MET:N	2.75	0.60
1:A:200:PRO:HG3	2:B:318:GLU:HB3	1.83	0.60
1:D:445:LEU:HD12	1:D:459:VAL:HG11	1.84	0.60
2:C:275:VAL:HG21	2:C:283:LYS:HZ2	1.66	0.60
3:F:66:ARG:HE	3:F:67:MET:HE2	1.66	0.60
1:D:391:LYS:O	1:D:430:ASN:ND2	2.34	0.60
3:E:472:THR:HG23	3:E:492:SER:HB3	1.83	0.60
1:A:264:LEU:HD21	1:A:267:GLU:HB2	1.84	0.59
1:A:329:MET:SD	1:A:329:MET:N	2.75	0.59
1:A:578:VAL:HG21	1:A:621:LEU:HG	1.84	0.59
1:D:233:ASN:CB	2:C:78:LEU:HD12	2.28	0.59
1:D:251:LEU:HD21	1:D:378:PHE:HB2	1.84	0.59
2:B:372:ALA:HA	2:B:375:MET:HE2	1.83	0.59
2:C:68:PHE:CE1	2:C:406:GLY:HA3	2.38	0.59
2:C:584:ILE:HG21	2:C:590:LEU:HD21	1.83	0.59
3:E:393:LEU:N	3:E:417:CYS:SG	2.75	0.59
3:E:704:THR:HB	3:E:707:ALA:HB3	1.85	0.59
1:A:241:TYR:OH	4:G:10:PRO:HB3	2.03	0.59
2:C:704:PRO:HA	3:F:744:GLN:HG3	1.85	0.59
3:F:552:PRO:HB2	3:F:554:LEU:HG	1.83	0.59
1:A:45:CYS:O	1:A:48:PHE:HB3	2.01	0.59
1:A:90:PHE:HB2	1:A:123:LEU:HD21	1.85	0.59
1:A:690:ARG:NH1	2:B:2:GLU:HB3	2.11	0.59
1:D:90:PHE:HB2	1:D:123:LEU:HD21	1.84	0.59
3:F:614:VAL:HG13	3:F:651:GLY:HA3	1.84	0.59
1:D:640:GLU:HB3	2:C:236:GLY:HA2	1.84	0.59
1:A:445:LEU:HD12	1:A:459:VAL:HG11	1.84	0.59
2:B:487:LEU:HG	2:B:488:PRO:HD2	1.85	0.59
2:C:106:PHE:HB3	2:C:327:ILE:HG23	1.85	0.59
3:F:281:ILE:HD11	3:F:438:LYS:HB2	1.83	0.59
3:F:704:THR:HB	3:F:707:ALA:HB3	1.84	0.59
1:D:110:LYS:HG2	1:D:111:ALA:H	1.68	0.59
3:E:552:PRO:HB2	3:E:554:LEU:HG	1.84	0.59
1:D:637:SER:HB2	2:C:238:LEU:HA	1.84	0.59
1:D:649:ILE:HD11	1:D:674:ILE:HD13	1.84	0.59
2:C:31:SER:HB3	2:C:240:ARG:CD	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:692:ARG:HG3	3:F:694:PRO:HD2	1.85	0.59
1:A:110:LYS:HG2	1:A:111:ALA:H	1.68	0.58
1:A:649:ILE:HD11	1:A:674:ILE:HD13	1.84	0.58
3:F:148:GLN:HB3	3:F:504:ASP:OD2	2.03	0.58
3:F:393:LEU:N	3:F:417:CYS:SG	2.76	0.58
3:F:438:LYS:HG3	3:F:441:ARG:HB2	1.85	0.58
1:A:180:GLU:O	1:A:183:ILE:HG13	2.03	0.58
2:B:665:ARG:HD2	3:E:89:VAL:HG21	1.85	0.58
1:D:236:LEU:CD1	2:C:480:LEU:HD22	2.27	0.58
2:B:68:PHE:CE1	2:B:406:GLY:HA3	2.38	0.58
2:B:290:SER:HB2	3:E:374:GLU:OE2	2.04	0.58
2:B:424:THR:HG22	2:B:474:ILE:HD11	1.84	0.58
1:A:654:GLU:HA	1:A:657:LYS:HB2	1.85	0.58
1:D:419:ASN:ND2	2:C:543:SER:OG	2.37	0.58
2:C:487:LEU:HG	2:C:488:PRO:HD2	1.85	0.58
3:E:148:GLN:HB3	3:E:504:ASP:OD2	2.04	0.58
2:C:424:THR:HG22	2:C:474:ILE:HD11	1.84	0.58
1:D:140:LYS:HZ3	1:D:145:PRO:HD2	1.67	0.58
1:D:473:GLU:HG3	1:D:475:LEU:HG	1.86	0.58
1:A:251:LEU:HD21	1:A:378:PHE:HB2	1.84	0.58
1:D:214:GLU:OE1	2:C:336:LYS:NZ	2.36	0.58
2:B:356:GLY:HA2	2:B:375:MET:HE1	1.86	0.58
1:D:264:LEU:HD21	1:D:267:GLU:HB2	1.84	0.58
1:D:242:GLU:N	1:D:242:GLU:OE1	2.37	0.58
3:F:342:LEU:HD23	3:F:377:GLY:HA2	1.86	0.58
1:A:412:GLU:HG2	2:B:601:ASN:ND2	2.19	0.58
2:C:631:PRO:O	3:F:64:ASN:HB2	2.04	0.58
3:E:438:LYS:HG3	3:E:441:ARG:HB2	1.85	0.58
3:F:390:GLU:O	3:F:391:ARG:HG2	2.04	0.58
3:F:716:GLU:O	3:F:749:THR:OG1	2.18	0.58
2:B:439:TRP:HB2	2:B:450:LEU:HD11	1.86	0.57
3:E:342:LEU:HD23	3:E:377:GLY:HA2	1.86	0.57
1:A:233:ASN:HB2	2:B:78:LEU:HD12	1.86	0.57
1:A:642:PHE:HE2	1:A:687:MET:HB2	1.67	0.57
1:D:412:GLU:HG2	2:C:601:ASN:CG	2.28	0.57
1:D:642:PHE:HE2	1:D:687:MET:HB2	1.68	0.57
3:E:390:GLU:O	3:E:391:ARG:HG2	2.04	0.57
3:E:614:VAL:HG13	3:E:651:GLY:HA3	1.85	0.57
1:A:140:LYS:HZ3	1:A:145:PRO:HD2	1.66	0.57
1:A:174:PHE:HB3	1:A:179:GLU:HB3	1.86	0.57
3:E:479:SER:O	3:E:498:ILE:N	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:439:TRP:HB2	2:C:450:LEU:HD11	1.85	0.57
3:E:414:MET:HE3	3:E:467:ARG:HE	1.69	0.57
3:F:414:MET:HE3	3:F:467:ARG:HE	1.70	0.57
2:B:542:PRO:HG3	3:E:247:TRP:HE1	1.69	0.57
2:B:106:PHE:HB3	2:B:327:ILE:HG23	1.85	0.57
2:C:356:GLY:HA2	2:C:375:MET:HE1	1.86	0.57
2:C:683:LYS:O	2:C:686:GLN:HB2	2.05	0.57
3:F:324:LYS:HZ1	3:F:331:LEU:HD22	1.66	0.57
1:A:583:LEU:HB3	3:E:246:THR:HG21	1.87	0.57
3:E:147:ARG:N	3:E:227:VAL:O	2.33	0.57
1:D:183:ILE:HD13	2:C:334:LEU:HD22	1.86	0.57
2:B:424:THR:HG21	2:B:476:ILE:HD12	1.87	0.57
2:C:49:TYR:HE2	2:C:310:LYS:HG2	1.70	0.56
2:C:623:ASN:ND2	3:F:113:ASN:H	2.03	0.56
1:A:45:CYS:HB3	1:A:94:ILE:HD11	1.87	0.56
1:A:398:TRP:CG	1:A:433:ARG:HA	2.41	0.56
1:A:651:MET:HE1	2:B:490:LEU:HD22	1.88	0.56
1:D:165:ARG:HD3	2:C:706:GLY:HA2	1.88	0.56
1:D:341:GLY:N	1:D:503:THR:HG21	2.20	0.56
1:D:355:LEU:HD22	1:D:358:ASP:HB3	1.86	0.56
3:E:76:GLU:OE2	3:E:80:VAL:HB	2.05	0.56
3:F:124:SER:HB2	3:F:128:ARG:HH21	1.71	0.56
1:A:355:LEU:HD22	1:A:358:ASP:HB3	1.87	0.56
1:D:45:CYS:HB3	1:D:94:ILE:HD11	1.87	0.56
1:A:261:HIS:CD2	1:A:265:MET:HE3	2.41	0.56
2:C:188:THR:HA	2:C:207:PRO:HA	1.88	0.56
3:E:124:SER:HB2	3:E:128:ARG:HH21	1.71	0.56
3:E:692:ARG:HG3	3:E:694:PRO:HD2	1.86	0.56
1:D:34:LYS:HZ1	1:D:180:GLU:CD	2.14	0.56
1:D:59:ASP:OD2	3:F:769:LYS:NZ	2.38	0.56
1:D:566:LYS:HG3	3:F:52:ARG:HH12	1.71	0.56
1:A:54:SER:HB2	1:A:60:ARG:NE	2.20	0.56
1:D:291:LYS:HD3	1:D:324:ILE:HG22	1.87	0.56
1:D:398:TRP:CG	1:D:433:ARG:HA	2.41	0.56
3:E:196:MET:HE3	3:E:218:PHE:HZ	1.71	0.56
3:E:324:LYS:HZ1	3:E:331:LEU:HD22	1.71	0.56
3:F:76:GLU:OE2	3:F:80:VAL:HB	2.06	0.56
3:F:391:ARG:HH22	3:F:423:PHE:HZ	1.53	0.56
3:F:620:ARG:NH2	3:F:644:THR:O	2.39	0.56
1:D:174:PHE:HB3	1:D:179:GLU:HB3	1.86	0.55
1:D:274:ILE:HA	1:D:481:MET:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:GLY:O	2:B:316:GLN:NE2	2.39	0.55
2:C:83:GLY:O	2:C:316:GLN:NE2	2.40	0.55
3:F:147:ARG:N	3:F:227:VAL:O	2.33	0.55
1:A:274:ILE:HA	1:A:481:MET:HB3	1.88	0.55
1:D:281:ARG:HD3	2:C:570:LYS:HB3	1.87	0.55
2:B:49:TYR:HE2	2:B:310:LYS:HG2	1.70	0.55
2:B:275:VAL:HG21	2:B:283:LYS:HZ1	1.70	0.55
2:C:523:ASP:OD2	2:C:560:TYR:OH	2.21	0.55
2:B:188:THR:HA	2:B:207:PRO:HA	1.88	0.55
3:E:381:SER:HB2	3:E:405:ASP:OD2	2.07	0.55
1:D:236:LEU:HD11	2:C:480:LEU:CD2	2.30	0.55
2:C:424:THR:HG21	2:C:476:ILE:HD12	1.87	0.55
2:C:438:PHE:HB2	2:C:453:VAL:HB	1.88	0.55
3:E:713:SER:HB3	3:E:753:THR:HG21	1.89	0.55
1:A:238:ILE:CD1	1:A:663:PHE:HB2	2.35	0.55
3:E:620:ARG:NH2	3:E:644:THR:O	2.39	0.55
3:E:716:GLU:O	3:E:749:THR:OG1	2.18	0.55
3:F:713:SER:HB3	3:F:753:THR:HG21	1.88	0.55
1:A:310:PRO:HD2	3:F:134:GLU:OE2	2.06	0.55
2:B:610:GLU:O	2:B:614:PHE:HB2	2.07	0.55
2:C:61:PHE:HE2	2:C:348:ASN:HD22	1.55	0.55
1:A:34:LYS:NZ	1:A:180:GLU:OE1	2.39	0.55
3:F:393:LEU:HD22	3:F:396:ILE:HD11	1.89	0.55
1:A:291:LYS:HD3	1:A:324:ILE:HG22	1.87	0.55
1:D:261:HIS:CD2	1:D:265:MET:HE3	2.42	0.55
3:E:391:ARG:HH22	3:E:423:PHE:HZ	1.53	0.55
3:F:472:THR:HG23	3:F:492:SER:HB3	1.89	0.55
1:A:47:MET:O	1:A:152:ARG:NH1	2.40	0.54
1:A:467:GLU:HB3	1:A:479:SER:HB2	1.89	0.54
1:D:419:ASN:O	1:D:423:GLU:HB2	2.07	0.54
1:D:562:ASP:HB2	3:F:49:LEU:HD13	1.89	0.54
3:E:393:LEU:HD22	3:E:396:ILE:HD11	1.89	0.54
1:D:331:ILE:C	1:D:332:ASN:HD22	2.15	0.54
3:F:197:ARG:NH1	3:F:703:ASP:O	2.39	0.54
3:E:189:ASN:ND2	3:E:308:GLU:OE1	2.40	0.54
3:E:197:ARG:NH1	3:E:703:ASP:O	2.39	0.54
1:A:176:PRO:O	1:A:180:GLU:HB3	2.06	0.54
1:A:419:ASN:O	1:A:423:GLU:HB2	2.07	0.54
1:D:47:MET:O	1:D:152:ARG:NH1	2.40	0.54
2:B:294:ARG:HG3	3:E:395:TRP:CH2	2.41	0.54
3:F:189:ASN:ND2	3:F:308:GLU:OE1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ARG:HD3	2:B:570:LYS:HB3	1.89	0.54
3:F:381:SER:HB2	3:F:405:ASP:OD2	2.07	0.54
1:D:467:GLU:HB3	1:D:479:SER:HB2	1.88	0.54
1:A:287:ILE:HA	1:A:290:PHE:HB2	1.90	0.54
1:A:331:ILE:C	1:A:332:ASN:HD22	2.15	0.54
1:D:165:ARG:HE	1:D:170:PHE:HZ	1.55	0.54
2:C:577:ILE:HA	2:C:580:PHE:HB3	1.90	0.54
2:C:610:GLU:O	2:C:614:PHE:HB2	2.07	0.54
2:C:708:MET:HG3	3:F:745:GLY:O	2.07	0.54
1:A:226:LYS:HD2	2:B:466:ARG:NE	2.23	0.54
1:A:183:ILE:HB	2:B:334:LEU:HD13	1.90	0.54
1:A:239:LYS:HZ3	4:G:6:PRO:HB2	1.73	0.54
1:A:341:GLY:N	1:A:503:THR:HG21	2.23	0.54
1:A:409:ASN:OD1	1:A:409:ASN:N	2.41	0.54
1:D:287:ILE:HA	1:D:290:PHE:HB2	1.90	0.54
2:C:688:VAL:HG22	3:F:24:MET:HE3	1.89	0.54
3:F:371:GLU:O	3:F:389:LYS:HA	2.08	0.54
1:A:49:CYS:SG	1:A:50:ASP:N	2.82	0.53
2:C:134:TRP:HZ3	2:C:183:PHE:CE1	2.26	0.53
3:E:194:LYS:O	3:E:198:SER:HB3	2.07	0.53
1:A:25:VAL:HG21	1:A:35:ILE:HG22	1.90	0.53
1:D:25:VAL:HG21	1:D:35:ILE:HG22	1.90	0.53
1:D:409:ASN:OD1	1:D:409:ASN:N	2.40	0.53
2:B:515:THR:O	3:E:48:SER:HB2	2.08	0.53
3:F:196:MET:HE3	3:F:218:PHE:HZ	1.72	0.53
1:A:239:LYS:HZ1	4:G:6:PRO:CD	2.20	0.53
1:D:112:ASP:N	1:D:112:ASP:OD1	2.42	0.53
2:B:134:TRP:HZ3	2:B:183:PHE:CE1	2.26	0.53
2:B:577:ILE:HA	2:B:580:PHE:HB3	1.91	0.53
3:F:658:PHE:O	3:F:664:PHE:HA	2.08	0.53
3:F:741:PHE:HA	3:F:747:VAL:HG22	1.91	0.53
1:A:640:GLU:OE2	2:B:29:PRO:HD3	2.08	0.53
1:D:145:PRO:O	1:D:150:LYS:HE3	2.09	0.53
2:B:523:ASP:OD2	2:B:560:TYR:OH	2.22	0.53
3:E:50:ARG:HH11	3:E:53:TRP:CD1	2.27	0.53
3:E:349:GLY:HA3	3:E:371:GLU:HG2	1.91	0.53
1:A:109:ARG:NH1	1:A:171:ASN:OD1	2.40	0.53
1:A:112:ASP:OD1	1:A:112:ASP:N	2.41	0.53
1:A:210:LYS:HG3	2:B:336:LYS:HZ1	1.73	0.53
2:C:44:LYS:O	2:C:48:ASP:HB2	2.09	0.53
3:E:158:GLU:HG3	3:E:159:GLN:HG3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:453:ILE:HG12	3:E:463:LEU:HD22	1.91	0.53
3:E:626:GLN:O	3:E:632:TYR:HB3	2.09	0.53
3:E:658:PHE:O	3:E:664:PHE:HA	2.08	0.53
3:F:158:GLU:HG3	3:F:159:GLN:HG3	1.91	0.53
3:F:194:LYS:O	3:F:198:SER:HB3	2.08	0.53
1:A:273:LYS:NZ	1:A:286:LEU:HD12	2.24	0.53
3:E:369:TRP:HH2	3:E:528:ARG:HA	1.74	0.53
1:A:341:GLY:H	1:A:503:THR:HG21	1.74	0.52
1:D:273:LYS:NZ	1:D:286:LEU:HD12	2.24	0.52
2:B:44:LYS:O	2:B:48:ASP:HB2	2.09	0.52
3:E:741:PHE:HA	3:E:747:VAL:HG22	1.90	0.52
3:F:626:GLN:O	3:F:632:TYR:HB3	2.09	0.52
1:D:171:ASN:ND2	2:C:167:GLU:OE2	2.41	0.52
1:D:401:MET:HE1	2:C:551:ILE:HD11	1.91	0.52
2:B:314:CYS:SG	2:B:477:ASN:ND2	2.82	0.52
3:F:565:THR:HG22	3:F:685:TYR:HB3	1.91	0.52
1:A:223:LEU:HB2	2:B:432:LEU:HD21	1.91	0.52
1:D:660:LYS:HB3	2:C:487:LEU:HB3	1.92	0.52
2:C:314:CYS:SG	2:C:477:ASN:ND2	2.82	0.52
1:D:366:LYS:NZ	2:C:368:VAL:HG23	2.24	0.52
2:B:357:ILE:O	2:B:370:ILE:HG22	2.10	0.52
3:E:565:THR:HG22	3:E:685:TYR:HB3	1.90	0.52
1:D:640:GLU:OE1	2:C:236:GLY:N	2.42	0.52
3:F:349:GLY:HA3	3:F:371:GLU:HG2	1.91	0.52
1:A:355:LEU:HG	2:B:368:VAL:HG11	1.91	0.52
2:B:71:CYS:O	2:B:84:ASN:ND2	2.42	0.52
2:C:357:ILE:O	2:C:370:ILE:HG22	2.09	0.52
3:E:371:GLU:O	3:E:389:LYS:HA	2.09	0.52
2:C:493:PHE:O	2:C:496:MET:HB2	2.10	0.52
3:E:514:LEU:HB2	3:E:524:ASP:HA	1.92	0.52
1:A:145:PRO:O	1:A:150:LYS:HE3	2.09	0.52
3:E:39:THR:HG22	3:E:40:THR:N	2.24	0.52
3:F:741:PHE:CE2	3:F:745:GLY:HA2	2.45	0.52
1:A:531:THR:HG21	3:F:669:VAL:HG13	1.92	0.51
1:D:586:SER:HB3	1:D:593:LEU:HB2	1.92	0.51
3:E:121:VAL:HG22	3:E:200:PHE:HE1	1.75	0.51
3:F:42:ARG:H	3:F:42:ARG:HD2	1.75	0.51
3:F:154:THR:HG22	3:F:236:MET:HB3	1.93	0.51
3:F:682:SER:HA	3:F:691:ILE:HB	1.92	0.51
2:B:535:MET:HG2	3:E:247:TRP:HH2	1.75	0.51
2:C:468:ASN:O	2:C:468:ASN:ND2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:682:SER:HA	3:E:691:ILE:HB	1.92	0.51
3:F:410:LEU:HD11	3:F:481:MET:HE3	1.93	0.51
1:A:165:ARG:HE	1:A:170:PHE:HZ	1.56	0.51
1:A:529:HIS:H	1:A:529:HIS:HD1	1.58	0.51
2:C:279:GLU:HG2	3:F:149:ARG:HD2	1.91	0.51
2:C:506:LEU:HD12	2:C:540:LEU:HD22	1.93	0.51
2:B:61:PHE:HE2	2:B:348:ASN:HD22	1.56	0.51
2:B:65:ARG:NH2	2:B:348:ASN:HD21	2.01	0.51
2:B:506:LEU:HD12	2:B:540:LEU:HD22	1.93	0.51
2:C:668:ARG:HH22	3:F:89:VAL:H	1.59	0.51
3:E:741:PHE:CE2	3:E:745:GLY:HA2	2.46	0.51
3:F:121:VAL:HG22	3:F:200:PHE:HE1	1.75	0.51
2:C:71:CYS:O	2:C:84:ASN:ND2	2.43	0.51
1:A:453:PRO:HA	1:A:493:SER:OG	2.11	0.51
2:B:468:ASN:O	2:B:468:ASN:ND2	2.43	0.51
3:F:228:PHE:CE2	3:F:235:ARG:NH1	2.59	0.51
1:D:176:PRO:O	1:D:180:GLU:HB3	2.10	0.51
2:B:520:GLU:HG2	2:B:560:TYR:CE2	2.46	0.51
1:A:586:SER:HB3	1:A:593:LEU:HB2	1.93	0.51
1:D:155:SER:HB3	3:F:713:SER:OG	2.10	0.51
1:D:317:TRP:CD1	1:D:321:LYS:HD2	2.46	0.51
2:B:55:GLU:HG3	2:B:66:ARG:HG3	1.93	0.51
2:B:624:ARG:NH1	3:E:107:PHE:O	2.42	0.51
3:F:369:TRP:HH2	3:F:528:ARG:HA	1.74	0.51
1:A:140:LYS:HE2	1:A:145:PRO:HD2	1.93	0.51
3:E:651:GLY:C	3:E:653:PHE:H	2.19	0.51
1:D:183:ILE:HD13	2:C:334:LEU:HD13	1.93	0.51
2:B:105:PHE:HE2	2:B:264:ILE:HG23	1.76	0.51
2:C:520:GLU:HG2	2:C:560:TYR:CE2	2.46	0.51
2:C:688:VAL:HG13	3:F:24:MET:HE2	1.92	0.51
3:E:277:ALA:HA	3:E:287:LYS:HD3	1.93	0.51
2:B:708:MET:HG3	3:E:745:GLY:O	2.11	0.50
2:C:55:GLU:HG3	2:C:66:ARG:HG3	1.93	0.50
2:C:454:ALA:HB3	2:C:460:ILE:HG12	1.93	0.50
3:E:160:ARG:HE	3:E:263:LYS:HZ2	1.59	0.50
3:F:266:ILE:HG12	3:F:297:MET:HE3	1.93	0.50
3:F:514:LEU:HB2	3:F:524:ASP:HA	1.92	0.50
1:A:113:ASP:O	1:A:117:GLN:HG2	2.11	0.50
1:A:317:TRP:CD1	1:A:321:LYS:HD2	2.46	0.50
1:D:33:ARG:H	1:D:33:ARG:HD2	1.76	0.50
1:D:453:PRO:HA	1:D:493:SER:OG	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:660:LYS:HZ3	2:C:489:GLU:HB2	1.76	0.50
3:E:416:PHE:HA	3:E:446:GLN:NE2	2.26	0.50
3:F:416:PHE:HA	3:F:446:GLN:NE2	2.26	0.50
3:F:453:ILE:HG12	3:F:463:LEU:HD22	1.91	0.50
1:A:275:SER:HB3	1:A:482:ASP:OD2	2.11	0.50
2:C:432:LEU:CD2	2:C:466:ARG:HH12	2.25	0.50
3:E:42:ARG:H	3:E:42:ARG:HD2	1.76	0.50
3:E:324:LYS:HD3	3:E:331:LEU:HD13	1.94	0.50
3:F:324:LYS:HD3	3:F:331:LEU:HD13	1.94	0.50
1:A:183:ILE:HD13	2:B:334:LEU:CD2	2.41	0.50
1:D:233:ASN:HB2	2:C:78:LEU:CD1	2.34	0.50
1:D:396:THR:OG1	1:D:468:ARG:N	2.45	0.50
2:B:438:PHE:HB2	2:B:453:VAL:HB	1.92	0.50
2:C:105:PHE:HE2	2:C:264:ILE:HG23	1.76	0.50
2:B:493:PHE:O	2:B:496:MET:HB2	2.10	0.50
1:D:113:ASP:O	1:D:117:GLN:HG2	2.11	0.50
1:D:259:TYR:CE1	1:D:261:HIS:HB3	2.46	0.50
2:B:432:LEU:CD2	2:B:466:ARG:HH12	2.23	0.50
2:C:65:ARG:NH2	2:C:348:ASN:HD21	2.02	0.50
3:E:343:LYS:HE3	3:E:505:MET:HE2	1.93	0.50
1:D:238:ILE:CD1	1:D:663:PHE:HB2	2.39	0.50
1:D:514:PRO:HG3	1:D:524:VAL:HG11	1.94	0.50
1:A:267:GLU:OE1	1:A:267:GLU:N	2.42	0.50
1:D:115:TYR:CD1	1:D:175:LEU:HD13	2.47	0.50
1:A:299:ARG:NE	3:F:545:GLN:HE22	2.08	0.50
3:E:154:THR:HG22	3:E:236:MET:HB3	1.92	0.50
3:F:277:ALA:HA	3:F:287:LYS:HD3	1.94	0.50
3:F:651:GLY:C	3:F:653:PHE:H	2.20	0.50
1:A:33:ARG:HH22	1:A:183:ILE:HG21	1.76	0.49
1:A:635:ASN:HA	1:A:639:LEU:HD23	1.94	0.49
1:D:34:LYS:NZ	1:D:180:GLU:OE1	2.39	0.49
1:D:275:SER:HB3	1:D:482:ASP:OD2	2.11	0.49
1:D:405:PRO:HG2	2:C:601:ASN:ND2	2.26	0.49
2:C:304:ILE:HG22	2:C:485:GLY:HA3	1.94	0.49
1:D:635:ASN:HA	1:D:639:LEU:HD23	1.94	0.49
3:E:244:GLY:HA3	3:E:247:TRP:HE3	1.77	0.49
3:F:343:LYS:HE3	3:F:505:MET:HE2	1.93	0.49
3:E:591:TYR:CD1	3:E:627:VAL:HG21	2.48	0.49
1:A:60:ARG:HD2	1:A:98:GLU:HB2	1.94	0.49
1:A:115:TYR:CD1	1:A:175:LEU:HD13	2.47	0.49
2:C:686:GLN:NE2	3:F:39:THR:OG1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LYS:HE2	1:D:145:PRO:HD2	1.93	0.49
2:B:454:ALA:HB3	2:B:460:ILE:HG12	1.94	0.49
3:E:317:SER:HB3	3:E:320:VAL:HG23	1.95	0.49
3:F:39:THR:HG22	3:F:40:THR:N	2.28	0.49
3:F:591:TYR:CD1	3:F:627:VAL:HG21	2.48	0.49
1:A:514:PRO:HG3	1:A:524:VAL:HG11	1.93	0.49
2:C:496:MET:HG2	2:C:503:VAL:HG11	1.95	0.49
2:C:707:ALA:O	2:C:708:MET:HG2	2.13	0.49
3:E:410:LEU:HD11	3:E:481:MET:HE3	1.93	0.49
3:F:244:GLY:HA3	3:F:247:TRP:HE3	1.78	0.49
1:D:410:GLU:OE1	1:D:410:GLU:C	2.48	0.49
2:B:496:MET:HG2	2:B:503:VAL:HG11	1.94	0.49
3:E:266:ILE:HG12	3:E:297:MET:HE3	1.93	0.49
3:E:734:PHE:HA	3:E:752:ARG:HB2	1.95	0.49
3:F:734:PHE:HA	3:F:752:ARG:HB2	1.95	0.49
1:A:499:ASP:OD2	2:B:30:MET:CE	2.61	0.49
2:B:302:VAL:HG11	2:B:460:ILE:HG21	1.94	0.49
3:F:176:GLU:HB2	3:F:197:ARG:HH21	1.77	0.49
1:A:364:GLY:O	2:B:361:ASN:HB3	2.13	0.49
1:D:33:ARG:HH12	1:D:183:ILE:HG21	1.78	0.49
2:B:432:LEU:HD23	2:B:466:ARG:NH1	2.26	0.49
3:E:176:GLU:HB2	3:E:197:ARG:HH21	1.78	0.49
1:A:403:GLU:OE2	1:A:403:GLU:N	2.44	0.48
2:B:52:THR:HG22	2:B:54:VAL:N	2.24	0.48
3:E:39:THR:HG22	3:E:40:THR:OG1	2.13	0.48
1:D:267:GLU:OE1	1:D:267:GLU:N	2.42	0.48
2:B:665:ARG:HE	3:E:60:PRO:HA	1.78	0.48
2:C:462:TRP:NE1	2:C:466:ARG:HD2	2.28	0.48
3:E:122:TYR:CE1	3:E:213:MET:HG2	2.48	0.48
2:B:462:TRP:NE1	2:B:466:ARG:HD2	2.29	0.48
2:C:4:ASN:HB3	2:C:7:LEU:HG	1.94	0.48
3:F:122:TYR:CE1	3:F:213:MET:HG2	2.48	0.48
1:D:109:ARG:NH1	1:D:171:ASN:OD1	2.40	0.48
1:D:236:LEU:HD21	2:C:480:LEU:HD13	1.95	0.48
2:B:22:TYR:CD2	2:B:24:TYR:HE2	2.27	0.48
2:C:432:LEU:HD23	2:C:466:ARG:NH1	2.27	0.48
2:C:606:HIS:NE2	3:F:128:ARG:HD3	2.28	0.48
3:E:406:ARG:HB3	3:E:481:MET:HE1	1.96	0.48
3:F:479:SER:O	3:F:498:ILE:N	2.28	0.48
2:B:304:ILE:HG22	2:B:485:GLY:HA3	1.94	0.48
1:A:416:GLU:HG2	1:A:420:LYS:HE2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:GLU:N	1:D:403:GLU:OE2	2.44	0.48
1:A:410:GLU:OE1	1:A:410:GLU:C	2.48	0.48
1:D:356:THR:HG22	2:C:377:LYS:NZ	2.28	0.48
1:A:691:LEU:O	1:A:695:VAL:HG23	2.13	0.48
1:D:477:VAL:HG23	1:D:478:PRO:O	2.13	0.48
1:D:691:LEU:O	1:D:695:VAL:HG23	2.13	0.48
2:B:4:ASN:HB3	2:B:7:LEU:HG	1.94	0.48
2:B:350:PHE:HB3	2:B:401:VAL:CG2	2.44	0.48
2:C:286:THR:CG2	3:F:504:ASP:HB2	2.44	0.48
3:F:422:TYR:CE1	3:F:449:MET:HG3	2.48	0.48
1:A:5:PHE:HD2	2:B:111:MET:HE3	1.78	0.48
1:A:259:TYR:CE1	1:A:261:HIS:HB3	2.45	0.48
2:C:427:TYR:HD2	2:C:430:GLU:HB2	1.79	0.48
3:E:422:TYR:CE1	3:E:449:MET:HG3	2.48	0.48
1:D:416:GLU:HG2	1:D:420:LYS:HE2	1.94	0.47
1:D:518:LYS:HE3	1:D:519:HIS:CE1	2.48	0.47
1:D:665:PHE:HB2	2:C:480:LEU:O	2.14	0.47
2:B:613:LYS:O	2:B:617:MET:HG3	2.14	0.47
1:A:509:PHE:HB3	1:A:547:LEU:HD11	1.97	0.47
1:A:518:LYS:HE3	1:A:519:HIS:CE1	2.49	0.47
1:D:226:LYS:HZ3	2:C:431:GLU:HG3	1.77	0.47
1:D:467:GLU:HB2	1:D:481:MET:HE2	1.95	0.47
2:C:522:VAL:HG22	2:C:655:ALA:HB1	1.97	0.47
3:E:88:ASP:OD1	3:E:88:ASP:N	2.45	0.47
3:E:288:LEU:O	3:E:292:ILE:HG12	2.14	0.47
3:E:444:PRO:O	3:E:448:VAL:HG23	2.15	0.47
1:D:226:LYS:HZ1	2:C:431:GLU:HG3	1.77	0.47
1:D:509:PHE:HB3	1:D:547:LEU:HD11	1.96	0.47
2:B:680:ALA:HA	2:B:683:LYS:HE3	1.96	0.47
3:E:357:TYR:O	3:E:423:PHE:HB3	2.14	0.47
1:A:352:GLU:HG3	2:B:370:ILE:CD1	2.44	0.47
2:C:613:LYS:O	2:C:617:MET:HG3	2.14	0.47
3:F:388:ARG:HB3	3:F:388:ARG:NH1	2.30	0.47
3:F:444:PRO:O	3:F:448:VAL:HG23	2.15	0.47
1:A:317:TRP:O	1:A:321:LYS:HG3	2.14	0.47
1:D:660:LYS:HZ3	2:C:489:GLU:CB	2.27	0.47
2:B:68:PHE:HE1	2:B:406:GLY:HA3	1.78	0.47
2:B:427:TYR:HD2	2:B:430:GLU:HB2	1.79	0.47
2:B:707:ALA:O	2:B:708:MET:HG2	2.14	0.47
3:F:288:LEU:O	3:F:292:ILE:HG12	2.15	0.47
3:F:741:PHE:CZ	3:F:745:GLY:HA2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASP:O	1:A:52:TYR:N	2.48	0.47
1:D:317:TRP:O	1:D:321:LYS:HG3	2.15	0.47
1:D:593:LEU:O	1:D:597:THR:N	2.33	0.47
2:B:522:VAL:HG22	2:B:655:ALA:HB1	1.97	0.47
2:C:22:TYR:CD2	2:C:24:TYR:HE2	2.26	0.47
2:C:68:PHE:HE1	2:C:406:GLY:HA3	1.79	0.47
2:C:660:HIS:HE1	3:F:106:ASN:ND2	2.13	0.47
3:E:742:VAL:HB	3:E:746:SER:O	2.15	0.47
3:F:317:SER:HB3	3:F:320:VAL:HG23	1.94	0.47
3:F:357:TYR:O	3:F:423:PHE:HB3	2.14	0.47
3:F:632:TYR:OH	3:F:697:VAL:HB	2.15	0.47
3:F:742:VAL:HB	3:F:746:SER:O	2.15	0.47
1:A:176:PRO:HA	1:A:180:GLU:HB2	1.97	0.47
1:A:239:LYS:NZ	4:G:6:PRO:HB2	2.29	0.47
1:A:405:PRO:HG2	2:B:601:ASN:ND2	2.30	0.47
2:C:359:LEU:HB2	2:C:368:VAL:HB	1.97	0.47
3:E:632:TYR:OH	3:E:697:VAL:HB	2.15	0.47
3:E:741:PHE:CZ	3:E:745:GLY:HA2	2.50	0.47
1:A:326:ASP:OD1	1:A:327:ARG:N	2.46	0.47
1:D:33:ARG:H	1:D:33:ARG:CD	2.28	0.47
1:D:631:PHE:CD1	2:C:23:PRO:HB3	2.50	0.47
2:B:221:ILE:O	2:B:225:THR:OG1	2.23	0.47
2:B:304:ILE:HG12	2:B:450:LEU:HD23	1.96	0.47
2:B:359:LEU:HB2	2:B:368:VAL:HB	1.97	0.47
2:C:680:ALA:HA	2:C:683:LYS:HE3	1.96	0.47
3:E:368:TYR:HD2	3:E:391:ARG:HB3	1.79	0.47
1:A:10:GLU:HB2	3:E:330:GLN:HE22	1.79	0.47
1:A:151:LEU:HA	3:E:714:VAL:O	2.15	0.47
1:D:434:GLU:HB3	1:D:629:PHE:CE2	2.50	0.47
3:F:718:ASP:CG	3:F:719:PRO:HD3	2.40	0.47
1:D:278:GLU:O	1:D:281:ARG:HG2	2.16	0.46
1:D:317:TRP:NE1	1:D:321:LYS:HD2	2.30	0.46
2:B:503:VAL:O	2:B:503:VAL:HG22	2.15	0.46
2:C:270:GLU:OE1	2:C:270:GLU:N	2.39	0.46
2:C:282:ALA:HB2	3:F:148:GLN:HG2	1.97	0.46
2:C:503:VAL:HG22	2:C:503:VAL:O	2.15	0.46
2:B:557:ARG:HD3	2:B:563:HIS:HA	1.97	0.46
3:E:151:ARG:HA	3:E:223:ARG:O	2.15	0.46
3:E:718:ASP:CG	3:E:719:PRO:HD3	2.40	0.46
3:F:151:ARG:HB2	3:F:507:GLU:OE2	2.16	0.46
1:A:34:LYS:NZ	1:A:180:GLU:CD	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:HD22	2:B:543:SER:HG	1.62	0.46
1:A:434:GLU:HB3	1:A:629:PHE:CE2	2.51	0.46
1:D:54:SER:HB2	1:D:60:ARG:HG3	1.96	0.46
2:B:265:CYS:HB3	2:B:274:PRO:HD3	1.97	0.46
3:E:388:ARG:NH1	3:E:388:ARG:HB3	2.30	0.46
3:F:335:LEU:CB	3:F:342:LEU:O	2.64	0.46
3:F:406:ARG:HB3	3:F:481:MET:HE1	1.96	0.46
3:F:416:PHE:HA	3:F:446:GLN:HE21	1.81	0.46
1:A:368:SER:HB2	2:B:359:LEU:HD23	1.97	0.46
1:A:467:GLU:HB2	1:A:481:MET:HE2	1.97	0.46
2:B:450:LEU:HD22	2:B:467:PHE:CD2	2.51	0.46
3:F:416:PHE:HD1	3:F:446:GLN:HE22	1.62	0.46
1:A:317:TRP:NE1	1:A:321:LYS:HD2	2.31	0.46
1:A:402:ALA:HB1	1:A:403:GLU:OE2	2.16	0.46
2:C:628:PRO:HG2	3:F:205:LEU:HB3	1.98	0.46
3:F:147:ARG:HG2	3:F:150:ARG:HD3	1.98	0.46
3:F:151:ARG:HA	3:F:223:ARG:O	2.15	0.46
3:F:479:SER:HB2	3:F:497:THR:HB	1.97	0.46
3:F:657:LEU:H	3:F:657:LEU:HD23	1.81	0.46
1:A:222:GLU:O	1:A:226:LYS:HB2	2.15	0.46
1:A:299:ARG:NH2	3:F:300:GLY:O	2.49	0.46
1:A:469:LYS:HB3	1:A:469:LYS:HE2	1.69	0.46
3:F:161:LEU:HD12	3:F:165:GLU:HG3	1.98	0.46
3:F:373:GLU:O	3:F:387:SER:HA	2.16	0.46
3:F:412:MET:HE3	3:F:412:MET:HB3	1.73	0.46
1:A:402:ALA:HB3	2:B:550:ARG:HG2	1.98	0.46
1:D:414:TYR:CE2	2:C:542:PRO:HG2	2.46	0.46
2:C:515:THR:O	3:F:48:SER:HB2	2.16	0.46
3:E:335:LEU:CB	3:E:342:LEU:O	2.64	0.46
3:E:416:PHE:HD1	3:E:446:GLN:HE22	1.63	0.46
1:A:593:LEU:O	1:A:597:THR:N	2.33	0.46
2:C:654:GLU:HB3	3:F:125:ARG:HE	1.80	0.46
1:A:278:GLU:O	1:A:281:ARG:HG2	2.16	0.45
1:D:201:LEU:HD21	2:C:87:ILE:HD11	1.97	0.45
1:D:227:VAL:HG23	2:C:466:ARG:HH21	1.80	0.45
1:D:287:ILE:HG23	1:D:460:PRO:HB3	1.98	0.45
2:C:304:ILE:HG12	2:C:450:LEU:HD23	1.98	0.45
1:A:7:GLU:HG3	3:E:511:LYS:HD2	1.98	0.45
1:D:34:LYS:NZ	1:D:180:GLU:CD	2.73	0.45
1:D:222:GLU:O	1:D:226:LYS:HB2	2.15	0.45
1:D:440:LEU:HD22	1:D:462:TYR:HE2	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:THR:HA	2:C:73:GLU:HB2	1.97	0.45
2:C:710:ILE:HG13	3:F:29:VAL:HA	1.99	0.45
3:E:134:GLU:O	3:E:135:ILE:HG23	2.17	0.45
3:E:147:ARG:HG2	3:E:150:ARG:HD3	1.97	0.45
3:E:151:ARG:HB2	3:E:507:GLU:OE2	2.15	0.45
1:D:165:ARG:HG3	1:D:170:PHE:CZ	2.51	0.45
2:C:265:CYS:HB3	2:C:274:PRO:HD3	1.97	0.45
3:E:479:SER:HB2	3:E:497:THR:HB	1.97	0.45
3:F:134:GLU:O	3:F:135:ILE:HG23	2.17	0.45
3:F:269:VAL:HG21	3:F:297:MET:HE1	1.99	0.45
1:A:381:TRP:CG	1:A:518:LYS:HD3	2.52	0.45
1:D:381:TRP:CG	1:D:518:LYS:HD3	2.52	0.45
2:C:281:LYS:HB3	2:C:502:PHE:CE2	2.52	0.45
2:C:691:MET:HE2	3:F:11:TYR:HD2	1.81	0.45
3:E:340:MET:HE3	3:E:340:MET:HB2	1.86	0.45
1:A:165:ARG:HG3	1:A:170:PHE:CZ	2.51	0.45
1:A:239:LYS:HB2	1:A:242:GLU:HB3	1.98	0.45
2:B:49:TYR:CE2	2:B:310:LYS:HG2	2.51	0.45
2:C:557:ARG:HD3	2:C:563:HIS:HA	1.98	0.45
3:E:269:VAL:HG21	3:E:297:MET:HE1	1.98	0.45
3:E:122:TYR:O	3:E:125:ARG:N	2.50	0.45
3:E:161:LEU:HD12	3:E:165:GLU:HG3	1.98	0.45
3:F:368:TYR:HD2	3:F:391:ARG:HB3	1.80	0.45
3:F:469:ILE:HG22	3:F:493:LEU:HD13	1.99	0.45
2:C:428:MET:HG3	2:C:429:ASP:H	1.82	0.45
3:E:373:GLU:O	3:E:387:SER:HA	2.16	0.45
3:E:416:PHE:HA	3:E:446:GLN:HE21	1.81	0.45
3:E:721:ALA:HB1	3:E:738:VAL:HA	1.99	0.45
2:B:150:VAL:O	2:B:154:LYS:HG3	2.17	0.45
2:B:713:ALA:O	2:B:717:LYS:HB2	2.17	0.45
3:F:88:ASP:N	3:F:88:ASP:OD1	2.48	0.45
1:A:64:ILE:HG22	1:A:72:ALA:HB1	1.98	0.45
1:A:531:THR:HG21	3:F:669:VAL:HA	1.98	0.45
1:D:568:ARG:HB3	2:C:551:ILE:HD12	1.98	0.45
2:B:281:LYS:HB3	2:B:502:PHE:CE2	2.51	0.45
2:C:286:THR:HG23	3:F:504:ASP:HB2	1.99	0.45
3:E:335:LEU:HB3	3:E:342:LEU:HB2	1.99	0.45
3:E:595:TYR:CD2	3:E:620:ARG:NH1	2.85	0.45
3:F:122:TYR:O	3:F:125:ARG:N	2.50	0.45
3:F:721:ALA:HB1	3:F:738:VAL:HA	1.99	0.45
1:A:115:TYR:OH	1:A:119:LYS:NZ	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:CYS:CB	1:D:63:LEU:HD11	2.47	0.45
1:D:115:TYR:OH	1:D:119:LYS:NZ	2.31	0.45
1:D:559:ILE:HD12	1:D:559:ILE:H	1.82	0.45
2:C:350:PHE:HB3	2:C:401:VAL:CG2	2.44	0.45
2:C:420:LEU:O	2:C:424:THR:HG23	2.17	0.45
2:C:450:LEU:HD22	2:C:467:PHE:CD2	2.52	0.45
1:A:287:ILE:HG23	1:A:460:PRO:HB3	1.98	0.44
1:D:402:ALA:HB1	1:D:403:GLU:OE2	2.16	0.44
2:B:428:MET:HG3	2:B:429:ASP:H	1.82	0.44
2:C:576:ILE:CD1	3:F:100:SER:HB2	2.44	0.44
3:E:351:LYS:HE2	3:E:369:TRP:CZ2	2.53	0.44
3:F:230:ALA:HB3	3:F:235:ARG:HD2	1.98	0.44
1:A:194:LEU:HD11	2:B:348:ASN:CG	2.42	0.44
1:A:287:ILE:CG2	1:A:460:PRO:HB3	2.47	0.44
1:D:64:ILE:HG22	1:D:72:ALA:HB1	1.98	0.44
2:C:150:VAL:HG12	2:C:154:LYS:HE3	1.99	0.44
3:F:39:THR:HG22	3:F:40:THR:OG1	2.17	0.44
1:A:174:PHE:CD2	1:A:179:GLU:HB2	2.52	0.44
1:D:174:PHE:CD2	1:D:179:GLU:HB2	2.52	0.44
1:D:287:ILE:CG2	1:D:460:PRO:HB3	2.48	0.44
1:D:469:LYS:HB3	1:D:469:LYS:HE2	1.68	0.44
1:D:579:GLU:OE1	2:C:543:SER:HB3	2.17	0.44
2:C:52:THR:HG22	2:C:54:VAL:N	2.24	0.44
2:C:284:LEU:HG	2:C:442:LEU:HD22	1.99	0.44
2:C:663:ARG:HH21	3:F:40:THR:HG21	1.82	0.44
2:C:705:ILE:H	3:F:744:GLN:CB	2.29	0.44
3:E:657:LEU:HD23	3:E:657:LEU:H	1.81	0.44
3:F:739:ARG:HA	3:F:749:THR:HG22	1.99	0.44
2:C:535:MET:HG2	3:F:247:TRP:HH2	1.82	0.44
3:F:322:LEU:HD21	3:F:531:ALA:HB1	1.98	0.44
1:A:431:CYS:O	1:A:435:MET:HG3	2.18	0.44
1:D:248:GLN:HG3	1:D:249:ILE:H	1.82	0.44
2:B:671:LEU:HA	2:B:676:ARG:HB2	2.00	0.44
3:E:322:LEU:HD21	3:E:531:ALA:HB1	1.98	0.44
3:F:76:GLU:HB2	3:F:82:LEU:HG	1.99	0.44
3:F:419:ASP:CG	3:F:467:ARG:HH12	2.24	0.44
2:B:112:GLU:HB2	2:B:263:LYS:HG2	2.00	0.44
2:B:549:LEU:HD11	2:B:605:LEU:HD21	1.99	0.44
2:B:603:SER:HA	3:E:241:ALA:HB2	1.98	0.44
2:C:671:LEU:HA	2:C:676:ARG:HB2	2.00	0.44
2:C:713:ALA:O	2:C:717:LYS:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:324:LYS:HZ3	3:E:331:LEU:HD22	1.78	0.44
3:F:351:LYS:HE2	3:F:369:TRP:CZ2	2.52	0.44
1:A:109:ARG:NH1	1:A:171:ASN:HA	2.32	0.44
1:A:248:GLN:HG3	1:A:249:ILE:H	1.83	0.44
1:D:151:LEU:O	3:F:713:SER:OG	2.36	0.44
2:B:78:LEU:HD13	2:B:78:LEU:O	2.17	0.44
2:B:528:MET:HG2	2:B:549:LEU:HD21	2.00	0.44
1:D:109:ARG:NH1	1:D:171:ASN:HA	2.33	0.44
2:B:424:THR:CG2	2:B:474:ILE:HD11	2.47	0.44
2:C:686:GLN:OE1	3:F:39:THR:HG21	2.18	0.44
3:E:469:ILE:HG22	3:E:493:LEU:HD13	1.99	0.44
1:A:353:ILE:HD12	1:A:353:ILE:H	1.83	0.44
1:D:419:ASN:CG	2:C:550:ARG:HH22	2.25	0.44
1:D:431:CYS:O	1:D:435:MET:HG3	2.18	0.44
1:D:674:ILE:O	1:D:678:LEU:HD13	2.18	0.44
2:B:140:MET:HE2	2:B:675:MET:HE1	2.00	0.44
2:B:632:PHE:CD2	3:E:102:ILE:HG23	2.52	0.44
3:E:524:ASP:N	3:E:524:ASP:OD1	2.51	0.44
3:F:374:GLU:HG3	3:F:387:SER:HB3	2.00	0.44
1:A:467:GLU:N	1:A:479:SER:O	2.46	0.43
1:D:183:ILE:CD1	2:C:334:LEU:HD22	2.47	0.43
2:B:284:LEU:HG	2:B:442:LEU:HD22	1.98	0.43
2:B:436:GLY:O	2:B:454:ALA:HA	2.18	0.43
2:B:576:ILE:HD11	3:E:100:SER:HB2	2.00	0.43
2:C:549:LEU:HD11	2:C:605:LEU:HD21	1.99	0.43
3:E:244:GLY:HA3	3:E:247:TRP:CE3	2.53	0.43
3:F:595:TYR:CD2	3:F:620:ARG:NH1	2.86	0.43
1:A:239:LYS:HA	4:G:8:TYR:CE1	2.53	0.43
1:A:559:ILE:HD12	1:A:559:ILE:H	1.82	0.43
1:D:183:ILE:HD13	2:C:334:LEU:CD2	2.47	0.43
1:D:240:HIS:O	1:D:244:ASN:N	2.51	0.43
2:B:294:ARG:HG3	3:E:395:TRP:CZ2	2.53	0.43
2:C:150:VAL:O	2:C:154:LYS:HG3	2.17	0.43
3:E:412:MET:HB3	3:E:412:MET:HE3	1.73	0.43
3:F:335:LEU:HB3	3:F:342:LEU:HB2	1.99	0.43
3:F:684:ILE:HG12	3:F:689:ILE:HG12	2.00	0.43
1:A:200:PRO:CB	2:B:69:CYS:HB2	2.46	0.43
1:A:240:HIS:O	1:A:244:ASN:N	2.51	0.43
1:A:395:LEU:HB2	1:A:398:TRP:CZ2	2.53	0.43
1:A:674:ILE:O	1:A:678:LEU:HD13	2.18	0.43
2:B:181:ILE:HB	2:B:214:ILE:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LEU:O	2:B:424:THR:HG23	2.18	0.43
2:C:436:GLY:O	2:C:454:ALA:HA	2.19	0.43
3:E:684:ILE:HG12	3:E:689:ILE:HG12	2.00	0.43
3:E:739:ARG:HA	3:E:749:THR:HG22	1.99	0.43
3:F:139:GLU:N	3:F:139:GLU:OE1	2.52	0.43
3:F:244:GLY:HA3	3:F:247:TRP:CE3	2.53	0.43
3:F:763:VAL:O	3:F:767:VAL:HG23	2.18	0.43
1:A:646:GLN:HG2	1:A:650:LEU:HD23	2.00	0.43
1:D:35:ILE:HG13	1:D:36:ILE:N	2.33	0.43
1:D:295:LEU:O	1:D:298:ILE:HG22	2.18	0.43
1:D:326:ASP:OD1	1:D:327:ARG:N	2.46	0.43
2:C:528:MET:HG2	2:C:549:LEU:HD21	2.00	0.43
3:E:374:GLU:HG3	3:E:387:SER:HB3	2.00	0.43
3:F:169:LEU:HG	3:F:185:PHE:HE2	1.83	0.43
1:D:395:LEU:HB2	1:D:398:TRP:CZ2	2.54	0.43
1:D:637:SER:HB3	2:C:29:PRO:HB3	2.01	0.43
2:C:294:ARG:HG3	3:F:395:TRP:CZ2	2.53	0.43
2:C:424:THR:CG2	2:C:474:ILE:HD11	2.47	0.43
3:E:414:MET:HE1	3:E:463:LEU:O	2.19	0.43
3:F:163:THR:O	3:F:166:ILE:HG22	2.19	0.43
3:F:524:ASP:OD1	3:F:524:ASP:N	2.51	0.43
3:E:419:ASP:O	3:E:422:TYR:HB3	2.18	0.43
1:A:164:LEU:O	1:A:168:ASN:N	2.51	0.43
1:D:164:LEU:O	1:D:168:ASN:N	2.51	0.43
2:B:150:VAL:HG12	2:B:154:LYS:HE3	1.99	0.43
3:E:28:THR:OG1	3:E:29:VAL:N	2.52	0.43
3:E:147:ARG:HE	3:E:502:LYS:HG2	1.84	0.43
3:E:163:THR:O	3:E:166:ILE:HG22	2.19	0.43
1:A:355:LEU:HD12	2:B:378:TYR:OH	2.18	0.43
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.83	0.43
2:B:534:ASN:ND2	2:B:538:ASN:OD1	2.49	0.43
2:B:606:HIS:NE2	3:E:128:ARG:HD3	2.33	0.43
2:C:310:LYS:HD2	2:C:310:LYS:N	2.34	0.43
2:C:678:MET:HE3	2:C:678:MET:HB3	1.95	0.43
3:E:139:GLU:N	3:E:139:GLU:OE1	2.51	0.43
3:F:53:TRP:O	3:F:56:SER:OG	2.35	0.43
1:A:704:LYS:HD3	1:A:704:LYS:HA	1.61	0.43
2:B:722:ALA:HB1	2:B:736:TYR:CD2	2.54	0.43
2:C:112:GLU:HB2	2:C:263:LYS:HG2	2.00	0.43
2:C:128:GLY:HA3	2:C:251:ARG:NH2	2.33	0.43
3:F:119:LYS:HE2	3:F:119:LYS:HB3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:206:ASN:HB3	3:F:209:VAL:HB	2.00	0.43
1:D:364:GLY:O	2:C:361:ASN:HB3	2.18	0.43
1:D:566:LYS:NZ	3:F:52:ARG:HH11	2.17	0.43
2:B:77:GLU:H	2:B:77:GLU:HG2	1.68	0.43
2:B:420:LEU:O	2:B:423:SER:OG	2.23	0.43
2:C:181:ILE:HB	2:C:214:ILE:HG22	2.01	0.43
3:E:514:LEU:HD12	3:E:524:ASP:HA	2.01	0.43
3:E:595:TYR:CZ	3:E:620:ARG:HG3	2.54	0.43
3:F:549:PHE:CG	3:F:550:GLN:N	2.87	0.43
1:A:396:THR:OG1	1:A:468:ARG:N	2.52	0.42
1:D:140:LYS:CE	1:D:145:PRO:HD2	2.49	0.42
1:D:366:LYS:HZ3	2:C:368:VAL:HG23	1.83	0.42
2:B:705:ILE:H	3:E:744:GLN:CB	2.32	0.42
3:E:755:SER:O	3:E:757:ARG:HG3	2.19	0.42
3:F:419:ASP:O	3:F:422:TYR:HB3	2.19	0.42
1:A:419:ASN:OD1	2:B:547:MET:HE3	2.19	0.42
1:D:646:GLN:HG2	1:D:650:LEU:HD23	2.00	0.42
2:B:60:VAL:HG23	2:B:61:PHE:CD2	2.54	0.42
2:B:128:GLY:HA3	2:B:251:ARG:NH2	2.33	0.42
2:C:49:TYR:CE2	2:C:310:LYS:HG2	2.51	0.42
3:E:206:ASN:HB3	3:E:209:VAL:HB	2.00	0.42
3:E:228:PHE:CE1	3:E:243:GLY:HA3	2.53	0.42
3:F:514:LEU:HD12	3:F:524:ASP:HA	2.01	0.42
1:A:193:GLU:O	1:A:197:GLU:HG2	2.19	0.42
1:A:222:GLU:N	1:A:222:GLU:OE1	2.52	0.42
1:A:237:PRO:HG3	4:G:5:SEP:P	2.59	0.42
1:A:245:LYS:HA	1:A:706:PHE:HB2	2.02	0.42
1:A:400:PRO:O	1:A:568:ARG:NH2	2.47	0.42
2:B:275:VAL:HG21	2:B:283:LYS:HZ2	1.81	0.42
2:B:687:MET:O	2:B:691:MET:HB2	2.20	0.42
3:E:46:ASN:HB3	3:E:49:LEU:HB3	2.00	0.42
3:E:169:LEU:HG	3:E:185:PHE:HE2	1.83	0.42
3:E:535:ASP:OD1	3:E:536:LEU:N	2.52	0.42
3:E:733:GLY:O	3:E:752:ARG:HG3	2.19	0.42
3:F:138:LYS:HB3	3:F:250:GLU:HB2	2.02	0.42
3:F:340:MET:HE3	3:F:340:MET:HB2	1.86	0.42
1:A:35:ILE:HG13	1:A:36:ILE:N	2.34	0.42
1:A:88:LEU:HD21	1:A:126:SER:OG	2.19	0.42
1:A:176:PRO:HA	1:A:180:GLU:CB	2.50	0.42
1:A:273:LYS:HZ3	1:A:286:LEU:HD12	1.84	0.42
1:A:488:CYS:SG	1:A:504:ILE:HD11	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:GLU:OE1	1:D:222:GLU:N	2.52	0.42
1:D:400:PRO:O	1:D:568:ARG:NH2	2.46	0.42
2:C:60:VAL:HG23	2:C:61:PHE:CD2	2.54	0.42
2:C:140:MET:HE2	2:C:675:MET:HE1	2.00	0.42
2:C:311:TRP:CZ2	2:C:417:SER:HB3	2.54	0.42
3:E:419:ASP:CG	3:E:467:ARG:HH12	2.24	0.42
3:F:103:ASN:OD1	3:F:103:ASN:N	2.52	0.42
3:F:595:TYR:CZ	3:F:620:ARG:HG3	2.54	0.42
1:A:295:LEU:O	1:A:298:ILE:HG22	2.18	0.42
1:A:515:ASN:H	1:A:519:HIS:HD1	1.68	0.42
1:D:491:SER:OG	1:D:503:THR:OG1	2.28	0.42
2:B:248:MET:HE1	2:B:251:ARG:HD3	2.02	0.42
2:B:570:LYS:HE3	2:B:570:LYS:HB2	1.93	0.42
2:C:302:VAL:HG11	2:C:460:ILE:HG21	2.01	0.42
2:C:697:GLU:N	3:F:178:GLU:OE2	2.48	0.42
3:E:76:GLU:HB2	3:E:82:LEU:HG	2.00	0.42
2:B:294:ARG:HA	3:E:395:TRP:CE2	2.54	0.42
2:B:310:LYS:HD2	2:B:310:LYS:N	2.34	0.42
2:B:502:PHE:CD2	2:B:503:VAL:HG12	2.54	0.42
2:B:659:THR:HG23	2:B:660:HIS:ND1	2.35	0.42
2:C:660:HIS:HE1	3:F:106:ASN:HD21	1.68	0.42
3:E:549:PHE:CG	3:E:550:GLN:N	2.87	0.42
3:F:481:MET:SD	3:F:485:GLY:HA2	2.60	0.42
3:F:755:SER:O	3:F:757:ARG:HG3	2.19	0.42
1:A:452:PHE:CD1	1:A:457:LYS:HD2	2.54	0.42
2:B:128:GLY:HA3	2:B:251:ARG:HH21	1.85	0.42
2:B:362:LYS:HA	2:B:362:LYS:HD2	1.83	0.42
2:C:171:LYS:O	2:C:175:MET:HG3	2.19	0.42
2:C:705:ILE:H	3:F:744:GLN:HB2	1.85	0.42
3:E:103:ASN:N	3:E:103:ASN:OD1	2.52	0.42
3:E:376:TYR:CE2	3:E:505:MET:HG3	2.55	0.42
3:F:28:THR:OG1	3:F:29:VAL:N	2.52	0.42
3:F:169:LEU:HG	3:F:185:PHE:CE2	2.55	0.42
3:F:228:PHE:CE1	3:F:243:GLY:HA3	2.54	0.42
3:F:733:GLY:O	3:F:752:ARG:HG3	2.18	0.42
1:A:378:PHE:HA	1:A:379:PRO:HD3	1.95	0.42
1:A:426:LEU:HD21	1:A:621:LEU:HD22	2.02	0.42
1:D:174:PHE:HD1	1:D:175:LEU:H	1.67	0.42
1:D:193:GLU:O	1:D:197:GLU:HG2	2.19	0.42
2:B:46:THR:HG21	2:B:404:LEU:HD13	2.02	0.42
2:C:244:ALA:HB3	2:C:409:LEU:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:353:LYS:HG2	3:E:367:GLU:HG2	2.02	0.42
3:F:340:MET:CE	3:F:409:LEU:HD23	2.50	0.42
4:G:5:SEP:HA	4:G:6:PRO:HD3	1.79	0.42
1:A:466:LYS:HZ2	1:A:480:GLU:HB3	1.84	0.42
1:D:452:PHE:CD1	1:D:457:LYS:HD2	2.54	0.42
1:D:473:GLU:HG3	1:D:475:LEU:CG	2.49	0.42
2:C:275:VAL:HG21	2:C:283:LYS:HZ1	1.84	0.42
3:F:376:TYR:CE2	3:F:505:MET:HG3	2.55	0.42
1:A:499:ASP:OD2	2:B:30:MET:HE1	2.19	0.42
1:D:353:ILE:HD12	1:D:353:ILE:H	1.84	0.42
1:D:704:LYS:HA	1:D:704:LYS:HD3	1.61	0.42
2:B:171:LYS:O	2:B:175:MET:HG3	2.20	0.42
2:C:370:ILE:HD13	2:C:378:TYR:CZ	2.54	0.42
2:C:726:ARG:HD3	2:C:736:TYR:CG	2.55	0.42
3:E:272:LYS:NZ	3:E:542:VAL:H	2.18	0.42
3:E:734:PHE:HA	3:E:752:ARG:HG3	2.00	0.42
3:F:59:PHE:HZ	3:F:81:ALA:O	2.03	0.42
3:F:179:ALA:O	3:F:726:ARG:NH2	2.53	0.42
3:F:324:LYS:HZ3	3:F:331:LEU:HD22	1.82	0.42
3:F:414:MET:HE1	3:F:463:LEU:O	2.20	0.42
3:F:734:PHE:HA	3:F:752:ARG:HG3	2.00	0.42
1:A:140:LYS:CE	1:A:145:PRO:HD2	2.49	0.41
1:D:48:PHE:CD1	1:D:48:PHE:C	2.98	0.41
1:D:245:LYS:HA	1:D:706:PHE:HB2	2.02	0.41
2:B:168:TYR:O	2:B:172:MET:HG2	2.20	0.41
2:B:663:ARG:HH21	3:E:40:THR:HG21	1.84	0.41
2:C:46:THR:HG21	2:C:404:LEU:HD13	2.01	0.41
3:E:98:SER:OG	3:E:101:CYS:SG	2.75	0.41
3:E:562:THR:O	3:E:566:LYS:HB2	2.20	0.41
3:F:562:THR:O	3:F:566:LYS:HB2	2.20	0.41
1:D:88:LEU:HD21	1:D:126:SER:OG	2.19	0.41
1:D:378:PHE:HA	1:D:379:PRO:HD3	1.95	0.41
2:B:715:GLU:OE2	3:E:11:TYR:OH	2.19	0.41
2:C:231:LYS:HD2	2:C:231:LYS:HA	1.90	0.41
2:C:420:LEU:O	2:C:423:SER:OG	2.22	0.41
2:C:557:ARG:HB3	2:C:562:VAL:O	2.21	0.41
3:E:169:LEU:HG	3:E:185:PHE:CE2	2.55	0.41
3:E:472:THR:CG2	3:E:492:SER:HB3	2.50	0.41
3:F:19:LYS:O	3:F:23:MET:HG2	2.20	0.41
1:D:395:LEU:HB3	1:D:465:SER:OG	2.20	0.41
2:B:9:PHE:HD1	2:B:14:VAL:HG22	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:557:ARG:HB3	2:B:562:VAL:O	2.21	0.41
2:C:128:GLY:HA3	2:C:251:ARG:HH21	1.85	0.41
2:C:329:LYS:HG3	2:C:330:ASP:N	2.35	0.41
2:C:502:PHE:CD2	2:C:503:VAL:HG12	2.54	0.41
2:C:659:THR:HG23	2:C:660:HIS:ND1	2.35	0.41
1:A:4:THR:O	1:A:8:ILE:HG13	2.21	0.41
1:D:327:ARG:NE	1:D:329:MET:SD	2.94	0.41
1:D:488:CYS:SG	1:D:504:ILE:HD11	2.60	0.41
2:B:541:SER:HB2	2:B:542:PRO:HD2	2.01	0.41
3:E:603:MET:HE2	3:E:603:MET:HB3	1.96	0.41
1:A:123:LEU:HD13	1:A:127:CYS:SG	2.60	0.41
1:A:140:LYS:NZ	1:A:145:PRO:HD2	2.35	0.41
1:A:327:ARG:NE	1:A:329:MET:SD	2.94	0.41
1:A:441:THR:CG2	1:A:462:TYR:H	2.33	0.41
1:A:449:CYS:HA	1:A:490:LYS:NZ	2.36	0.41
2:B:244:ALA:HB3	2:B:409:LEU:HD13	2.02	0.41
2:B:311:TRP:CZ2	2:B:417:SER:HB3	2.54	0.41
2:B:329:LYS:HG3	2:B:330:ASP:N	2.35	0.41
3:E:481:MET:SD	3:E:485:GLY:HA2	2.60	0.41
3:E:517:SER:N	3:E:521:GLU:O	2.45	0.41
3:F:46:ASN:HB3	3:F:49:LEU:HB3	2.03	0.41
3:F:144:LEU:HD23	3:F:244:GLY:O	2.21	0.41
3:F:147:ARG:HE	3:F:502:LYS:HG2	1.84	0.41
1:D:515:ASN:H	1:D:519:HIS:HD1	1.68	0.41
2:C:93:LEU:HD12	2:C:474:ILE:HD13	2.03	0.41
3:E:179:ALA:O	3:E:726:ARG:NH2	2.53	0.41
3:F:490:ILE:HG22	3:F:491:LYS:HG3	2.03	0.41
1:A:49:CYS:CB	1:A:63:LEU:HD11	2.50	0.41
1:D:123:LEU:HD13	1:D:127:CYS:SG	2.61	0.41
1:D:440:LEU:HD22	1:D:462:TYR:CE2	2.56	0.41
1:D:638:GLN:HB3	1:D:677:CYS:O	2.21	0.41
2:B:722:ALA:HB1	2:B:736:TYR:HD2	1.86	0.41
2:C:359:LEU:O	2:C:367:GLU:HA	2.21	0.41
2:C:534:ASN:ND2	2:C:538:ASN:OD1	2.49	0.41
2:C:703:PRO:HA	2:C:704:PRO:HD3	1.97	0.41
3:E:197:ARG:O	3:E:201:ALA:CB	2.69	0.41
3:E:340:MET:CE	3:E:409:LEU:HD23	2.50	0.41
3:F:272:LYS:NZ	3:F:542:VAL:H	2.18	0.41
3:F:353:LYS:HG2	3:F:367:GLU:HG2	2.02	0.41
3:F:407:LYS:HD3	3:F:484:ASP:C	2.45	0.41
3:F:595:TYR:CE2	3:F:620:ARG:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.83	0.41
1:A:522:TYR:CZ	1:A:552:ARG:HD2	2.55	0.41
1:D:584:ARG:NH1	2:C:501:GLU:HG2	2.35	0.41
2:B:295:MET:SD	2:B:301:ALA:HB2	2.61	0.41
2:B:359:LEU:O	2:B:367:GLU:HA	2.20	0.41
2:B:686:GLN:OE1	3:E:39:THR:CG2	2.61	0.41
3:E:144:LEU:HD23	3:E:244:GLY:O	2.20	0.41
3:E:387:SER:HG	3:E:395:TRP:HE3	1.66	0.41
3:E:552:PRO:O	3:E:553:ASP:HB2	2.21	0.41
3:F:242:LEU:HD21	3:F:252:ASN:HD22	1.84	0.41
3:F:517:SER:N	3:F:521:GLU:O	2.45	0.41
1:A:48:PHE:CD1	1:A:48:PHE:C	2.99	0.41
1:A:214:GLU:OE1	2:B:336:LYS:NZ	2.54	0.41
1:A:236:LEU:CD1	2:B:480:LEU:HD22	2.47	0.41
1:A:395:LEU:HB3	1:A:465:SER:OG	2.20	0.41
1:A:457:LYS:HE2	1:A:457:LYS:HB3	1.90	0.41
1:D:176:PRO:HA	1:D:180:GLU:HB2	2.01	0.41
1:D:192:LEU:HD23	1:D:195:ARG:NH1	2.36	0.41
1:D:355:LEU:HG	2:C:368:VAL:HG11	2.03	0.41
1:D:522:TYR:CZ	1:D:552:ARG:HD2	2.55	0.41
2:B:370:ILE:HD13	2:B:378:TYR:CZ	2.55	0.41
2:C:295:MET:SD	2:C:301:ALA:HB2	2.61	0.41
2:C:304:ILE:HG13	2:C:450:LEU:HB3	2.02	0.41
2:C:342:ALA:HB3	2:C:343:PRO:HD3	2.03	0.41
3:E:59:PHE:HZ	3:E:81:ALA:O	2.03	0.41
3:E:407:LYS:HD3	3:E:484:ASP:C	2.45	0.41
3:E:490:ILE:HG22	3:E:491:LYS:HG3	2.02	0.41
3:F:197:ARG:O	3:F:201:ALA:CB	2.69	0.41
3:F:340:MET:HE2	3:F:409:LEU:HD23	2.02	0.41
1:A:414:TYR:HE2	2:B:542:PRO:HG2	1.86	0.41
2:B:24:TYR:CD2	2:B:507:ALA:HB1	2.56	0.41
2:B:570:LYS:HD3	2:B:575:LYS:NZ	2.36	0.41
2:C:168:TYR:O	2:C:172:MET:HG2	2.21	0.41
2:C:541:SER:HB2	2:C:542:PRO:HD2	2.02	0.41
3:E:467:ARG:HD3	3:E:467:ARG:HA	1.85	0.41
1:A:192:LEU:HD23	1:A:195:ARG:NH1	2.36	0.40
1:A:349:LYS:HA	2:B:367:GLU:O	2.21	0.40
1:A:644:ASN:O	1:A:647:LYS:HE2	2.21	0.40
1:D:4:THR:O	1:D:8:ILE:HG13	2.21	0.40
1:D:277:PRO:O	1:D:281:ARG:HB3	2.21	0.40
1:D:457:LYS:HE2	1:D:457:LYS:HB3	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:24:TYR:CD2	2:C:507:ALA:HB1	2.56	0.40
2:C:65:ARG:HG3	2:C:405:PRO:HG3	2.03	0.40
3:F:73:ILE:HG22	3:F:75:LYS:H	1.85	0.40
3:F:330:GLN:HG3	3:F:513:HIS:HB2	2.04	0.40
3:F:356:VAL:HG11	3:F:423:PHE:CD2	2.57	0.40
1:A:392:ASP:HA	1:A:429:THR:HA	2.02	0.40
1:D:392:ASP:HA	1:D:429:THR:HA	2.02	0.40
2:B:370:ILE:HD12	2:B:370:ILE:HA	1.80	0.40
2:B:628:PRO:HB3	3:E:206:ASN:OD1	2.22	0.40
2:C:248:MET:HE1	2:C:251:ARG:HD3	2.02	0.40
2:C:576:ILE:H	2:C:576:ILE:HG13	1.67	0.40
2:C:631:PRO:HG2	2:C:632:PHE:CE1	2.56	0.40
3:E:19:LYS:O	3:E:23:MET:HG2	2.21	0.40
3:E:76:GLU:HG2	3:E:77:HIS:H	1.87	0.40
3:E:330:GLN:HG3	3:E:513:HIS:HB2	2.03	0.40
3:F:705:SER:O	3:F:709:LEU:HD23	2.21	0.40
1:A:624:GLN:NE2	2:B:8:MET:SD	2.94	0.40
1:D:63:LEU:HD12	1:D:63:LEU:N	2.36	0.40
1:D:495:LEU:HD23	1:D:495:LEU:HA	1.86	0.40
3:E:382:ALA:HA	3:E:400:GLY:HA2	2.03	0.40
3:E:634:LEU:HD23	3:E:696:VAL:HA	2.03	0.40
3:E:705:SER:O	3:E:709:LEU:HD23	2.21	0.40
3:F:565:THR:CG2	3:F:685:TYR:HB3	2.52	0.40
1:A:638:GLN:HB3	1:A:677:CYS:O	2.21	0.40
1:D:333:GLU:HA	1:D:336:HIS:CE1	2.57	0.40
2:C:9:PHE:HD1	2:C:14:VAL:HG22	1.85	0.40
3:F:190:TYR:HE2	3:F:681:SER:HB2	1.87	0.40
3:F:244:GLY:N	3:F:247:TRP:HB2	2.37	0.40
3:F:535:ASP:OD1	3:F:536:LEU:N	2.52	0.40
1:A:47:MET:H	1:A:47:MET:HG3	1.58	0.40
1:A:71:THR:HG22	1:A:75:LEU:HD13	2.04	0.40
2:B:342:ALA:HB3	2:B:343:PRO:HD3	2.03	0.40
2:C:214:ILE:HD12	2:C:214:ILE:HA	1.97	0.40
2:C:404:LEU:HA	2:C:405:PRO:HD3	1.91	0.40
3:E:166:ILE:HD12	3:E:218:PHE:HB2	2.04	0.40
3:E:244:GLY:N	3:E:247:TRP:HB2	2.37	0.40
3:E:340:MET:HE2	3:E:409:LEU:HD23	2.02	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	706/709 (100%)	674 (96%)	31 (4%)	1 (0%)	48	81
1	D	706/709 (100%)	678 (96%)	27 (4%)	1 (0%)	48	81
2	B	702/754 (93%)	678 (97%)	23 (3%)	1 (0%)	48	81
2	C	715/754 (95%)	691 (97%)	23 (3%)	1 (0%)	48	81
3	E	769/774 (99%)	732 (95%)	35 (5%)	2 (0%)	36	70
3	F	769/774 (99%)	731 (95%)	36 (5%)	2 (0%)	36	70
4	G	8/28 (29%)	6 (75%)	1 (12%)	1 (12%)	0	4
5	H	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
All	All	4383/4512 (97%)	4196 (96%)	178 (4%)	9 (0%)	43	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	13	PRO
3	E	89	VAL
3	E	533	ILE
3	F	89	VAL
3	F	533	ILE
1	D	540	VAL
2	B	503	VAL
2	C	503	VAL
1	A	540	VAL

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	630/631 (100%)	630 (100%)	0	100	100
1	D	630/631 (100%)	630 (100%)	0	100	100
2	B	630/669 (94%)	630 (100%)	0	100	100
2	C	639/669 (96%)	639 (100%)	0	100	100
3	E	676/679 (100%)	676 (100%)	0	100	100
3	F	676/679 (100%)	676 (100%)	0	100	100
4	G	10/24 (42%)	10 (100%)	0	100	100
All	All	3891/3982 (98%)	3891 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	243	GLN
1	A	248	GLN
1	A	332	ASN
1	A	615	GLN
1	A	624	GLN
1	A	627	GLN
1	A	638	GLN
1	D	204	GLN
1	D	243	GLN
1	D	248	GLN
1	D	332	ASN
1	D	615	GLN
1	D	627	GLN
1	D	638	GLN
1	D	644	ASN
2	B	84	ASN
2	B	296	ASN
2	B	348	ASN
2	B	459	ASN
2	B	534	ASN
2	B	554	GLN
2	B	563	HIS
2	B	627	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	84	ASN
2	C	296	ASN
2	C	348	ASN
2	C	459	ASN
2	C	534	ASN
2	C	563	HIS
2	C	627	ASN
2	C	660	HIS
3	E	78	ASN
3	E	219	ASN
3	E	261	GLN
3	E	454	GLN
3	E	519	ASN
3	E	626	GLN
3	E	717	ASN
3	E	727	GLN
3	F	78	ASN
3	F	148	GLN
3	F	219	ASN
3	F	261	GLN
3	F	359	GLN
3	F	403	ASN
3	F	454	GLN
3	F	519	ASN
3	F	545	GLN
3	F	626	GLN
3	F	670	ASN
3	F	727	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	SEP	G	12	4	8,9,10	1.48	1 (12%)	7,12,14	2.32	2 (28%)
4	SEP	G	5	4	8,9,10	1.62	1 (12%)	7,12,14	1.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SEP	G	12	4	-	6/6/8/10	-
4	SEP	G	5	4	-	6/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	SEP	P-O1P	3.55	1.61	1.50
4	G	12	SEP	P-O1P	3.10	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	12	SEP	OG-CB-CA	5.12	113.13	108.14
4	G	12	SEP	O3P-P-OG	2.73	113.79	106.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	5	SEP	N-CA-CB-OG
4	G	5	SEP	C-CA-CB-OG
4	G	5	SEP	CB-OG-P-O2P
4	G	5	SEP	CB-OG-P-O3P
4	G	12	SEP	N-CA-CB-OG
4	G	12	SEP	C-CA-CB-OG
4	G	12	SEP	CB-OG-P-O2P
4	G	5	SEP	CB-OG-P-O1P
4	G	12	SEP	CB-OG-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	12	SEP	CB-OG-P-O3P
4	G	5	SEP	CA-CB-OG-P
4	G	12	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	12	SEP	2	0
4	G	5	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	708/709 (99%)	0.67	40 (5%)	30	27	65, 123, 199, 259	0
1	D	708/709 (99%)	0.71	50 (7%)	22	22	67, 140, 219, 293	0
2	B	710/754 (94%)	0.60	34 (4%)	35	31	63, 115, 202, 293	0
2	C	721/754 (95%)	0.57	38 (5%)	32	28	75, 135, 203, 265	0
3	E	771/774 (99%)	1.01	101 (13%)	7	10	71, 161, 254, 321	0
3	F	771/774 (99%)	0.92	84 (10%)	10	13	82, 161, 229, 299	0
4	G	10/28 (35%)	0.88	0	100	100	167, 181, 197, 197	0
5	H	0/10	-	-	-	-	-	-
All	All	4399/4512 (97%)	0.75	347 (7%)	18	20	63, 139, 226, 321	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	242	ALA	6.5
3	E	200	PHE	5.7
1	D	341	GLY	5.5
1	A	497	LYS	5.2
1	A	340	LEU	5.0
1	A	341	GLY	4.8
1	A	1	MET	4.7
1	A	336	HIS	4.7
1	A	498	ASP	4.7
2	C	230	ALA	4.7
3	E	696	VAL	4.4
3	F	148	GLN	4.3
3	E	204	PRO	4.3
1	A	499	ASP	4.2
1	D	182	ILE	4.1
2	C	242	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	696	VAL	4.1
3	E	542	VAL	4.1
2	B	670	LEU	4.0
1	D	342	GLY	4.0
3	F	702	MET	4.0
3	F	244	GLY	4.0
1	D	677	CYS	4.0
3	F	208	GLU	4.0
2	C	236	GLY	3.9
3	F	424	LYS	3.9
1	D	698	ALA	3.9
3	F	232	ARG	3.9
3	F	149	ARG	3.8
3	F	224	PHE	3.8
3	E	250	GLU	3.8
1	D	687	MET	3.8
3	E	571	LEU	3.8
3	F	170	GLN	3.8
3	E	447	TYR	3.8
3	E	703	ASP	3.8
3	E	149	ARG	3.7
3	F	1	MET	3.7
3	F	447	TYR	3.6
3	F	768	LYS	3.6
2	B	441	GLY	3.5
2	B	230	ALA	3.4
3	F	47	PRO	3.4
2	B	669	THR	3.4
3	E	366	PHE	3.4
2	B	658	SER	3.4
1	D	541	ILE	3.3
3	F	252	ASN	3.3
3	F	81	ALA	3.3
1	D	336	HIS	3.3
1	D	517	GLU	3.3
3	F	247	TRP	3.3
3	F	95	VAL	3.2
2	C	753	SER	3.2
2	C	434	ALA	3.2
1	D	635	ASN	3.2
3	E	478	GLY	3.2
1	A	32	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	3.2
1	A	541	ILE	3.2
3	F	555	ALA	3.1
3	E	689	ILE	3.1
3	F	243	GLY	3.1
1	D	451	LEU	3.1
1	A	30	ASP	3.0
3	E	47	PRO	3.0
3	F	444	PRO	3.0
2	B	753	SER	3.0
3	E	212	HIS	3.0
2	C	24	TYR	3.0
2	B	654	GLU	3.0
3	E	81	ALA	3.0
3	E	37	LYS	3.0
3	E	344	LYS	3.0
3	F	86	THR	3.0
3	E	258	ASN	3.0
3	E	312	GLU	3.0
3	E	555	ALA	3.0
3	E	573	LYS	3.0
2	C	231	LYS	3.0
2	C	670	LEU	2.9
3	E	196	MET	2.9
3	E	308	GLU	2.9
3	E	599	GLU	2.9
1	A	342	GLY	2.9
3	F	771	LYS	2.9
3	F	372	GLN	2.9
3	E	550	GLN	2.9
1	A	539	SER	2.9
3	E	253	THR	2.9
3	F	242	LEU	2.9
1	D	1	MET	2.9
2	B	673	THR	2.8
3	F	253	THR	2.8
1	A	677	CYS	2.8
3	E	252	ASN	2.8
2	B	437	CYS	2.8
3	E	91	LYS	2.8
3	E	215	GLU	2.8
1	D	502	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	522	VAL	2.8
1	D	284	GLU	2.8
2	B	626	PHE	2.8
3	E	361	VAL	2.7
1	D	494	HIS	2.7
2	C	273	LEU	2.7
1	A	176	PRO	2.7
1	D	114	SER	2.7
1	A	504	ILE	2.7
3	F	330	GLN	2.7
2	B	378	TYR	2.7
1	A	396	THR	2.7
3	E	622	LEU	2.7
3	F	348	SER	2.7
1	D	555	ALA	2.7
1	A	343	ILE	2.7
3	E	314	ASP	2.6
3	E	422	TYR	2.6
2	C	150	VAL	2.6
3	F	200	PHE	2.6
1	D	656	ASP	2.6
3	E	693	VAL	2.6
1	A	467	GLU	2.6
1	D	640	GLU	2.6
1	D	497	LYS	2.6
3	F	692	ARG	2.6
2	C	274	PRO	2.6
3	E	625	THR	2.6
3	E	434	ASP	2.6
2	C	443	GLN	2.6
2	B	205	LYS	2.6
3	F	572	ILE	2.6
1	D	111	ALA	2.6
3	F	90	SER	2.6
3	F	703	ASP	2.6
3	E	586	ILE	2.6
3	E	715	CYS	2.6
3	F	695	LEU	2.6
3	F	279	ALA	2.6
2	B	333	ASP	2.5
2	C	442	LEU	2.5
3	E	771	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	91	LYS	2.5
1	D	224	ALA	2.5
1	D	518	LYS	2.5
1	A	182	ILE	2.5
3	E	303	GLU	2.5
3	E	244	GLY	2.5
2	B	580	PHE	2.5
2	C	432	LEU	2.5
3	F	347	GLY	2.5
1	A	368	SER	2.5
2	C	458	SER	2.5
3	E	41	SER	2.5
3	E	374	GLU	2.5
3	E	539	ASP	2.5
2	B	28	PRO	2.5
1	A	468	ARG	2.5
3	E	141	ARG	2.5
2	C	669	THR	2.4
3	F	215	GLU	2.4
3	F	574	ARG	2.4
3	F	652	MET	2.4
3	E	216	LYS	2.4
2	B	430	GLU	2.4
3	E	359	GLN	2.4
3	F	443	ILE	2.4
1	D	55	THR	2.4
3	F	431	THR	2.4
2	B	127	GLU	2.4
3	E	274	CYS	2.4
2	C	237	LYS	2.4
1	D	113	ASP	2.4
3	F	254	ALA	2.4
1	D	649	ILE	2.4
3	F	685	TYR	2.4
1	A	284	GLU	2.4
3	E	755	SER	2.4
1	D	24	ALA	2.4
3	E	279	ALA	2.4
2	B	733	ASP	2.4
3	F	523	PHE	2.4
3	F	361	VAL	2.4
3	F	234	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	190	TYR	2.4
3	E	487	LYS	2.4
3	E	667	PRO	2.4
2	B	632	PHE	2.3
2	C	25	THR	2.3
3	E	185	PHE	2.3
3	E	587	ALA	2.3
3	F	201	ALA	2.3
3	F	228	PHE	2.3
3	E	746	SER	2.3
3	E	66	ARG	2.3
3	E	263	LYS	2.3
3	F	45	LYS	2.3
2	B	339	CYS	2.3
3	E	331	LEU	2.3
2	B	410	MET	2.3
3	F	216	LYS	2.3
3	F	769	LYS	2.3
3	E	425	ASP	2.3
3	F	93	ASP	2.3
2	C	610	GLU	2.3
2	C	666	ALA	2.3
3	E	446	GLN	2.3
1	D	2	SER	2.3
1	D	636	ASP	2.3
2	B	730	ALA	2.3
3	E	43	LYS	2.3
3	F	80	VAL	2.3
3	E	311	LEU	2.3
3	F	226	PRO	2.3
3	F	478	GLY	2.3
2	B	672	ASN	2.3
3	F	577	THR	2.3
1	D	285	ILE	2.3
1	A	283	GLY	2.3
3	E	563	ALA	2.3
3	E	372	GLN	2.3
2	C	437	CYS	2.3
3	E	189	ASN	2.3
3	E	163	THR	2.3
2	C	504	SER	2.3
1	D	570	CYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	455	LYS	2.2
2	C	32	HIS	2.2
3	E	559	ASP	2.2
3	F	425	ASP	2.2
3	E	621	LYS	2.2
3	F	140	LEU	2.2
1	D	337	SER	2.2
3	F	183	SER	2.2
3	E	116	GLU	2.2
1	D	343	ILE	2.2
3	E	708	LEU	2.2
1	A	282	ALA	2.2
3	F	298	ARG	2.2
2	C	701	ILE	2.2
1	A	53	LEU	2.2
1	D	181	THR	2.2
3	E	687	HIS	2.2
2	B	497	PHE	2.2
3	E	148	GLN	2.2
1	A	227	VAL	2.2
3	E	395	TRP	2.2
1	A	500	GLY	2.2
2	C	296	ASN	2.2
3	E	519	ASN	2.2
2	B	458	SER	2.2
3	E	75	LYS	2.2
3	E	358	ILE	2.2
1	A	101	GLN	2.2
1	D	476	PRO	2.2
2	C	511	PRO	2.2
3	F	514	LEU	2.2
3	F	687	HIS	2.2
2	C	620	GLN	2.2
3	F	176	GLU	2.2
3	F	367	GLU	2.2
3	F	88	ASP	2.1
3	F	751	LYS	2.1
2	C	241	ARG	2.1
3	E	247	TRP	2.1
3	F	495	ALA	2.1
3	E	260	ASP	2.1
3	F	174	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	541	LYS	2.1
2	C	206	VAL	2.1
3	F	160	ARG	2.1
1	A	231	GLN	2.1
3	E	710	GLU	2.1
3	F	105	TRP	2.1
3	F	360	GLY	2.1
1	D	504	ILE	2.1
1	D	535	LYS	2.1
1	D	564	LEU	2.1
2	C	183	PHE	2.1
3	E	293	LYS	2.1
3	E	439	LEU	2.1
1	A	496	ASN	2.1
2	B	380	ASN	2.1
3	F	52	ARG	2.1
1	A	2	SER	2.1
1	A	179	GLU	2.1
1	D	664	GLY	2.1
2	C	233	GLY	2.1
3	E	251	ALA	2.1
3	E	647	ALA	2.1
1	D	81	LYS	2.1
3	F	383	THR	2.1
1	D	6	ALA	2.1
2	C	433	LYS	2.1
3	E	522	ALA	2.1
2	B	86	ASP	2.1
3	E	417	CYS	2.1
3	E	702	MET	2.1
1	A	294	ASN	2.1
1	D	409	ASN	2.1
1	D	645	GLU	2.1
3	F	2	SER	2.1
3	E	259	VAL	2.1
2	B	13	ASP	2.1
1	D	340	LEU	2.1
3	F	192	LEU	2.1
3	F	225	LEU	2.1
1	A	339	PHE	2.1
1	A	147	GLU	2.1
3	E	110	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	41	SER	2.1
2	B	675	MET	2.0
3	E	23	MET	2.0
3	E	236	MET	2.0
3	E	298	ARG	2.0
1	D	50	ASP	2.0
1	D	177	ASP	2.0
1	A	494	HIS	2.0
1	D	331	ILE	2.0
3	E	170	GLN	2.0
3	E	700	GLU	2.0
2	C	412	MET	2.0
1	A	140	LYS	2.0
1	D	346	ALA	2.0
2	C	190	VAL	2.0
3	E	158	GLU	2.0
3	F	141	ARG	2.0
1	D	166	LYS	2.0
3	E	140	LEU	2.0
3	E	286	SER	2.0
3	F	660	SER	2.0
2	C	33	GLY	2.0
2	C	429	ASP	2.0
1	A	438	CYS	2.0
1	A	535	LYS	2.0
1	D	396	THR	2.0
2	B	428	MET	2.0
2	B	667	ASN	2.0
2	B	553	LEU	2.0
2	C	751	LEU	2.0
3	E	58	LYS	2.0
3	E	187	LEU	2.0
3	E	577	THR	2.0
3	F	308	GLU	2.0
3	F	331	LEU	2.0
2	C	31	SER	2.0
3	E	90	SER	2.0

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

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(Å ²)	Q<0.9
4	SEP	G	12	10/11	0.51	0.14	191,224,246,253	0
4	SEP	G	5	10/11	0.77	0.15	184,191,200,207	0

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(Å ²)	Q<0.9
6	MG	D	801	1/1	0.03	0.33	145,145,145,145	0
6	MG	A	801	1/1	0.26	0.24	103,103,103,103	0
6	MG	D	800	1/1	0.65	0.17	193,193,193,193	0
6	MG	A	800	1/1	0.85	0.15	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.