



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:49 AM UTC

PDB ID : 1T03 / pdb_00001t03
Title : HIV-1 reverse transcriptase crosslinked to tenofovir terminated template-primer (complex P)
Authors : Tuske, S.; Sarafianos, S.G.; Ding, J.; Arnold, E.
Deposited on : 2004-04-07
Resolution : 3.10 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:

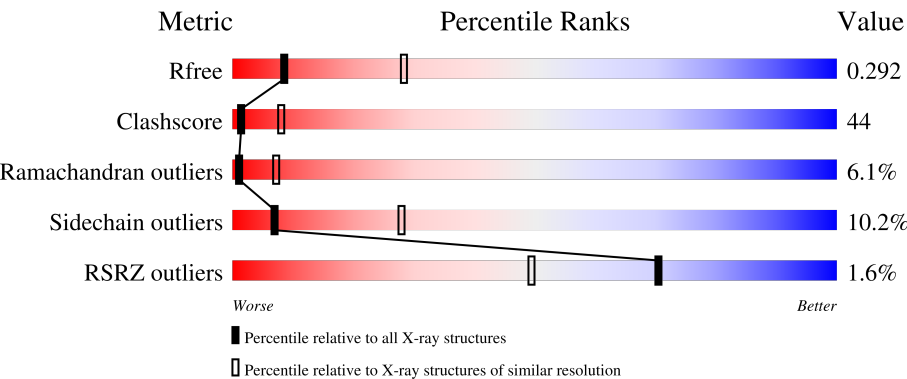
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	T	27	7% 33% 22% 30% 15%
2	P	21	5% 24% 48% 24% 5%
3	A	558	2% 38% 50% 11% .
4	B	437	% 33% 50% 14% ..
5	L	211	36% 55% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	225	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TFO	P	822[A]	-	X	-	X
2	TFO	P	822[B]	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12252 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 DNA chain called Synthetic oligonucleotide template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	23	Total	C	N	O	P	0	0	0
			473	223	95	133	22			

- Molecule 2 is a DNA chain called Synthetic oligonucleotide primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	20	Total	C	N	O	P	0	2	0
			434	209	80	125	20			

- Molecule 3 is a protein called POL polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	558	Total	C	N	O	S	15	0	0
			4482	2901	741	832	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 4 is a protein called POL polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	429	Total	C	N	O	S	4	0	0
			3534	2304	586	637	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
B	430	GLY	-	cloning artifact	UNP P03366

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	431	GLY	-	cloning artifact	UNP P03366
B	432	HIS	-	expression tag	UNP P03366
B	433	HIS	-	expression tag	UNP P03366
B	434	HIS	-	expression tag	UNP P03366
B	435	HIS	-	expression tag	UNP P03366
B	436	HIS	-	expression tag	UNP P03366
B	437	HIS	-	expression tag	UNP P03366

- Molecule 5 is a protein called monoclonal antibody light chain.

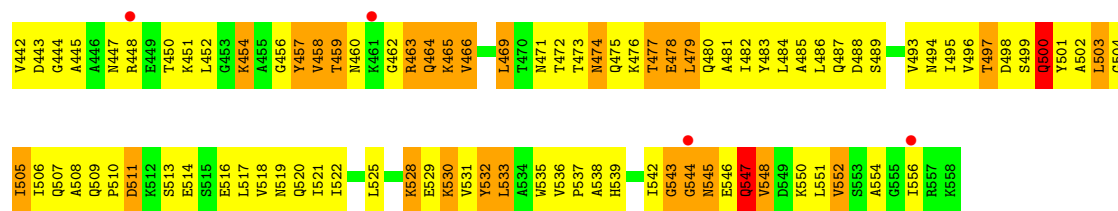
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	211	Total	C	N	O	S	0	0	0
			1643	1025	270	342	6			

- Molecule 6 is a protein called monoclonal antibody heavy chain.

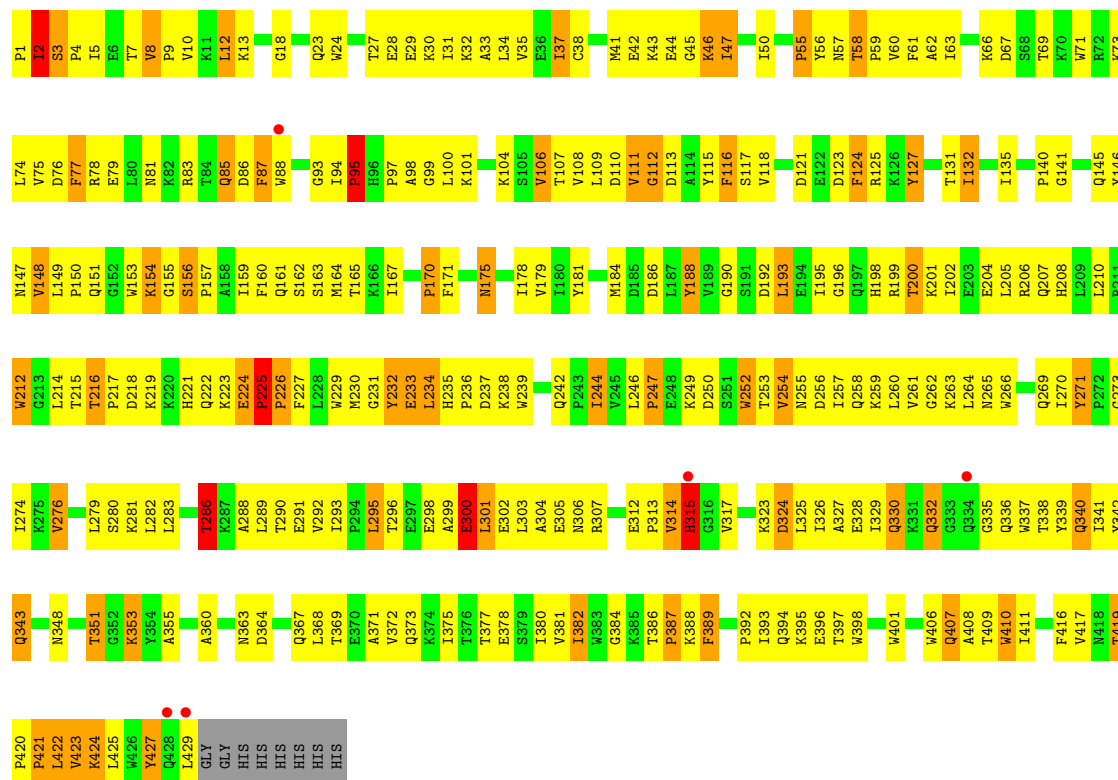
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	225	Total	C	N	O	S	0	0	0
			1685	1060	276	340	9			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

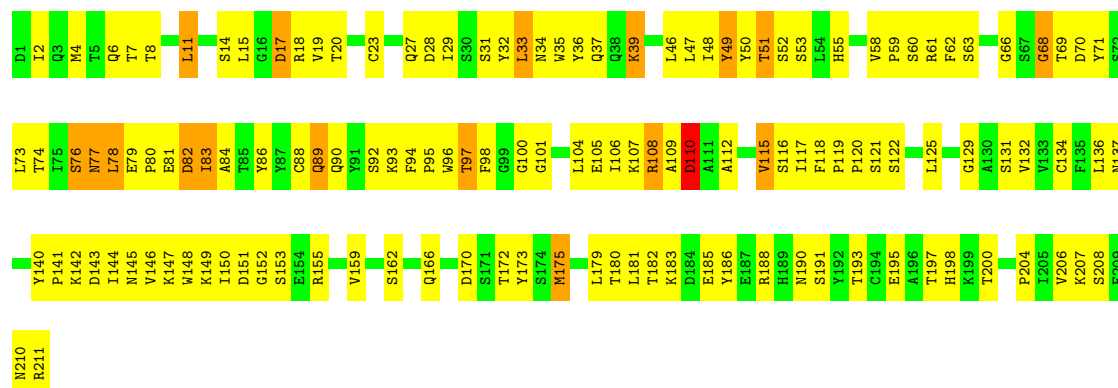
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		



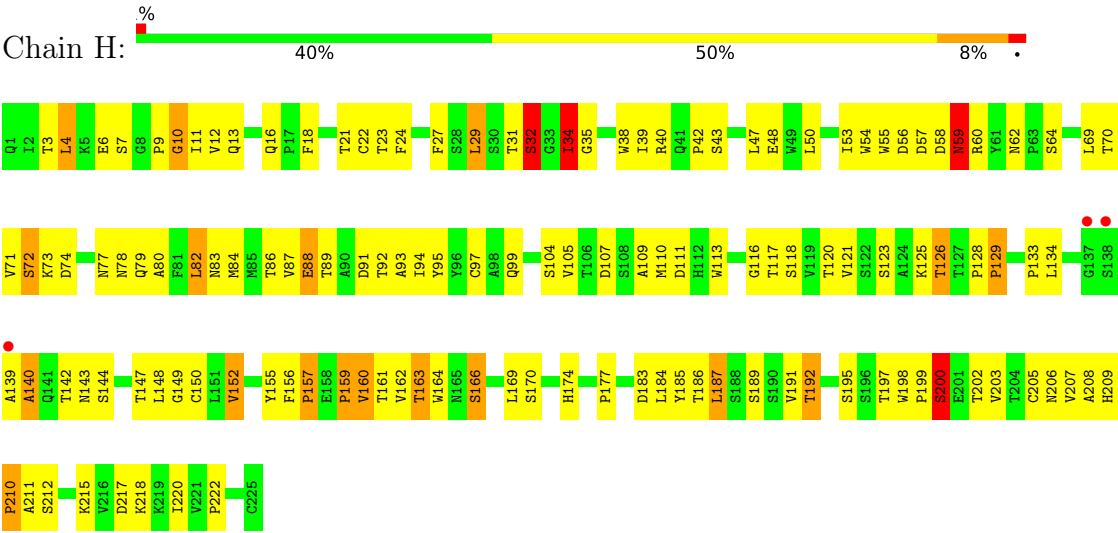
• Molecule 4: POL polypeptide



• Molecule 5: monoclonal antibody light chain



● Molecule 6: monoclonal antibody heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	166.78Å 166.78Å 221.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-3.10) 94.6 (20.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.256 , 0.295 0.251 , 0.292	Depositor DCC
R_{free} test set	2454 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.057 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12252	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: TFO, MG, MRG

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	T	0.43	0/532	1.06	12/820 (1.5%)
2	P	0.39	0/420	0.88	4/640 (0.6%)
3	A	0.53	0/4600	1.01	20/6259 (0.3%)
4	B	0.63	1/3639 (0.0%)	1.15	37/4949 (0.7%)
5	L	0.51	0/1681	1.05	7/2283 (0.3%)
6	H	0.61	0/1729	1.08	6/2372 (0.3%)
All	All	0.56	1/12601 (0.0%)	1.06	86/17323 (0.5%)

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
4	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	132	ILE	CA-CB	-6.07	1.49	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	86	ASP	N-CA-C	-12.51	97.31	111.82
4	B	427	TYR	N-CA-C	12.11	128.10	110.42
4	B	225	PRO	N-CA-C	11.32	124.51	110.70
3	A	365	VAL	N-CA-C	-10.60	100.54	110.82
1	T	705	DA	N9-C1'-C2'	-9.89	98.66	113.50
5	L	137	ASN	N-CA-C	9.55	124.94	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	382	ILE	N-CA-C	9.23	119.28	110.42
3	A	500	GLN	N-CA-C	-8.73	101.84	111.36
4	B	224	GLU	CA-C-N	8.51	129.15	120.38
4	B	224	GLU	C-N-CA	8.51	129.15	120.38
4	B	2	ILE	N-CA-C	7.63	125.20	109.34
3	A	3	SER	N-CA-C	7.61	119.66	110.07
1	T	705	DA	OP1-P-O3'	-7.30	86.08	108.00
4	B	8	VAL	CA-C-N	7.17	126.93	119.76
4	B	8	VAL	C-N-CA	7.17	126.93	119.76
4	B	88	TRP	N-CA-C	7.13	120.46	111.69
5	L	112	ALA	N-CA-C	7.08	118.98	110.07
1	T	712	DC	C2'-C3'-O3'	-6.92	101.12	111.50
4	B	291	GLU	N-CA-C	6.90	119.36	108.67
3	A	457	TYR	N-CA-C	6.88	120.75	109.94
1	T	713	DC	C2'-C3'-O3'	-6.84	101.24	111.50
3	A	391	LEU	N-CA-C	6.75	120.34	110.14
4	B	66	LYS	N-CA-C	-6.75	104.52	112.89
4	B	94	ILE	CA-C-N	6.64	128.14	119.84
4	B	94	ILE	C-N-CA	6.64	128.14	119.84
4	B	46	LYS	N-CA-C	-6.59	103.93	112.23
2	P	815	DG	C2'-C3'-O3'	-6.48	101.78	111.50
4	B	186	ASP	N-CA-C	6.45	119.52	109.52
3	A	118	VAL	CA-C-N	6.34	126.36	119.89
3	A	118	VAL	C-N-CA	6.34	126.36	119.89
1	T	711	DC	C2'-C3'-O3'	-6.25	102.12	111.50
3	A	320	ASP	CA-C-N	6.25	127.65	119.84
3	A	320	ASP	C-N-CA	6.25	127.65	119.84
4	B	343	GLN	N-CA-C	-6.22	105.34	113.12
4	B	112	GLY	N-CA-C	6.15	119.64	112.50
1	T	705	DA	O3'-P-O5'	-6.15	94.78	104.00
3	A	298	GLU	N-CA-C	-6.11	104.62	111.28
2	P	816	DG	C2'-C3'-O3'	-6.10	102.35	111.50
4	B	127	TYR	N-CA-C	6.10	118.72	111.71
5	L	100	GLY	N-CA-C	-6.10	105.19	115.80
5	L	186	TYR	N-CA-C	-6.08	104.56	111.07
3	A	349	LEU	N-CA-C	-5.92	103.51	112.04
2	P	818	DC	C2'-C3'-O3'	-5.89	102.66	111.50
5	L	115	VAL	N-CA-C	5.88	116.85	110.21
3	A	479	LEU	N-CA-C	-5.86	104.48	111.69
6	H	111	ASP	N-CA-C	5.76	118.30	111.33
2	P	815	DG	N9-C1'-C2'	5.76	122.14	113.50
3	A	79	GLU	N-CA-C	5.70	117.50	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	32	SER	N-CA-C	5.69	122.91	110.80
4	B	184	MET	CB-CA-C	-5.67	110.01	116.54
4	B	132	ILE	CA-C-N	5.59	126.38	120.11
4	B	132	ILE	C-N-CA	5.59	126.38	120.11
1	T	705	DA	C5'-C4'-C3'	-5.59	106.52	114.90
1	T	710	DG	C2'-C3'-O3'	-5.53	103.20	111.50
1	T	705	DA	OP2-P-O3'	-5.52	91.43	108.00
4	B	216	THR	CA-C-N	5.48	125.48	119.89
4	B	216	THR	C-N-CA	5.48	125.48	119.89
4	B	389	PHE	N-CA-C	5.47	118.15	109.24
3	A	224	GLU	CA-C-N	-5.46	114.76	120.38
3	A	224	GLU	C-N-CA	-5.46	114.76	120.38
3	A	184	MET	CB-CA-C	-5.44	110.32	116.63
6	H	29	LEU	N-CA-C	-5.40	106.88	112.93
3	A	436	GLY	N-CA-C	-5.35	107.24	116.01
5	L	175	MET	N-CA-C	5.34	116.28	107.20
4	B	252	TRP	N-CA-C	5.31	117.28	108.20
3	A	375	ILE	CB-CA-C	-5.30	105.09	111.88
5	L	105	GLU	N-CA-C	5.28	117.49	109.63
4	B	58	THR	CA-C-N	-5.25	113.89	120.51
4	B	58	THR	C-N-CA	-5.25	113.89	120.51
6	H	74	ASP	N-CA-C	-5.24	99.63	110.80
4	B	61	PHE	N-CA-C	-5.22	100.20	108.14
3	A	522	ILE	N-CA-C	-5.22	105.62	110.53
4	B	419	THR	CA-C-N	5.21	125.75	120.38
4	B	419	THR	C-N-CA	5.21	125.75	120.38
4	B	235	HIS	CA-C-N	5.19	126.33	119.84
4	B	235	HIS	C-N-CA	5.19	126.33	119.84
3	A	28	GLU	N-CA-C	-5.19	105.05	111.33
1	T	709	DC	C2'-C3'-O3'	-5.19	103.72	111.50
1	T	707	DG	C2'-C3'-O3'	-5.11	103.83	111.50
1	T	708	DG	C2'-C3'-O3'	-5.07	103.89	111.50
4	B	388	LYS	N-CA-C	-5.05	102.23	110.20
4	B	85	GLN	N-CA-C	5.04	121.55	110.80
6	H	140	ALA	N-CA-C	5.04	121.53	110.80
4	B	254	VAL	N-CA-C	-5.03	105.42	110.30
4	B	3	SER	N-CA-C	5.02	118.69	107.95
6	H	34	ILE	N-CA-C	5.01	119.76	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	188	TYR	Sidechain

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	T	473	0	257	32	0
2	P	434	0	248	23	0
3	A	4482	0	4485	430	0
4	B	3534	0	3568	329	1
5	L	1643	0	1565	165	0
6	H	1685	0	1640	127	0
7	A	1	0	0	0	0
All	All	12252	0	11763	1062	1

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 44.

All (1062) 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)
3:A:501:TYR:CE1	3:A:505:ILE:HD11	1.86	1.10
3:A:50:ILE:HD11	3:A:145:GLN:HB2	1.10	1.09
3:A:344:GLU:HG3	3:A:345:PRO:HD2	1.36	1.07
3:A:138:GLU:HG2	3:A:139:THR:H	1.10	1.06
5:L:61:ARG:HB2	5:L:76:SER:HB3	1.36	1.06
4:B:225:PRO:HB2	4:B:226:PRO:HD3	1.38	1.01
3:A:501:TYR:O	3:A:505:ILE:HG13	1.60	0.99
4:B:387:PRO:HG2	4:B:389:PHE:CE1	1.98	0.99
3:A:50:ILE:CD1	3:A:145:GLN:HB2	1.92	0.98
5:L:34:ASN:OD1	5:L:49:TYR:HA	1.62	0.98
5:L:136:LEU:HD22	5:L:175:MET:HE3	1.46	0.97
4:B:222:GLN:HG3	4:B:224:GLU:H	1.29	0.96
3:A:246:LEU:HD23	3:A:246:LEU:H	1.28	0.95
4:B:244:ILE:HD13	4:B:244:ILE:H	1.29	0.95
4:B:292:VAL:O	4:B:293:ILE:HD13	1.66	0.94
3:A:27:THR:OG1	3:A:30:LYS:HG3	1.68	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:4:MET:HE2	5:L:90:GLN:HB2	1.49	0.93
3:A:111:VAL:HG11	3:A:214:LEU:HD12	1.50	0.92
3:A:439:THR:HG21	4:B:289:LEU:H	1.34	0.92
5:L:83:ILE:HG21	5:L:106:ILE:HG23	1.52	0.92
4:B:257:ILE:O	4:B:261:VAL:HG23	1.71	0.91
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.51	0.90
6:H:92:THR:HG23	6:H:120:THR:HA	1.50	0.90
3:A:441:TYR:CE2	3:A:544:GLY:HA3	2.07	0.90
3:A:297:GLU:HA	3:A:300:GLU:HB2	1.55	0.88
3:A:3:SER:HB3	3:A:5:ILE:HG13	1.56	0.88
2:P:818:DC:H2'	2:P:819:DG:H8	1.39	0.88
5:L:34:ASN:HB2	5:L:89:GLN:NE2	1.89	0.87
5:L:120:PRO:HB2	5:L:125:LEU:HD21	1.54	0.87
3:A:279:LEU:HD23	3:A:279:LEU:H	1.38	0.87
3:A:22:LYS:H	3:A:22:LYS:HD3	1.38	0.86
3:A:11:LYS:H	3:A:85:GLN:HE21	1.19	0.86
3:A:443:ASP:O	3:A:481:ALA:HB2	1.74	0.86
3:A:466:VAL:HG12	3:A:466:VAL:O	1.75	0.86
4:B:222:GLN:HE21	4:B:224:GLU:HG3	1.41	0.85
5:L:23:CYS:SG	5:L:33:LEU:HD11	2.16	0.85
3:A:125:ARG:HG2	3:A:146:TYR:O	1.77	0.85
4:B:33:ALA:O	4:B:37:ILE:HG22	1.77	0.85
4:B:312:GLU:HB3	4:B:313:PRO:HD2	1.59	0.85
4:B:57:ASN:ND2	4:B:58:THR:H	1.75	0.84
5:L:34:ASN:HB2	5:L:89:GLN:HE21	1.43	0.84
5:L:34:ASN:HD22	5:L:89:GLN:HE22	1.26	0.84
4:B:254:VAL:HB	4:B:289:LEU:O	1.78	0.83
3:A:434:ILE:HG22	3:A:494:ASN:HD21	1.44	0.82
3:A:420:PRO:HG3	3:A:422:LEU:HG	1.62	0.82
5:L:195:GLU:HG2	5:L:206:VAL:HG22	1.61	0.82
6:H:69:LEU:HD21	6:H:84:MET:HE3	1.59	0.82
3:A:500:GLN:H	3:A:500:GLN:NE2	1.78	0.81
6:H:53:ILE:HB	6:H:71:VAL:HG11	1.61	0.81
3:A:244:ILE:HD11	3:A:263:LYS:HB3	1.62	0.81
4:B:237:ASP:C	4:B:239:TRP:H	1.85	0.81
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.10	0.81
3:A:478:GLU:OE1	3:A:498:ASP:OD1	1.99	0.81
3:A:344:GLU:CG	3:A:345:PRO:HD2	2.10	0.81
3:A:293:ILE:HD12	3:A:294:PRO:HD2	1.63	0.81
1:T:705:DA:H2	1:T:706:DT:H72	1.45	0.81
6:H:166:SER:N	6:H:206:ASN:HD21	1.78	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:454:LYS:HB2	3:A:454:LYS:NZ	1.96	0.80
6:H:62:ASN:HD21	6:H:64:SER:HB2	1.46	0.80
3:A:465:LYS:O	3:A:466:VAL:HG23	1.82	0.80
3:A:498:ASP:CB	3:A:538:ALA:HB2	2.12	0.80
4:B:279:LEU:HD11	4:B:302:GLU:HB2	1.62	0.80
4:B:2:ILE:HD12	4:B:3:SER:N	1.96	0.79
3:A:11:LYS:O	3:A:85:GLN:HG2	1.82	0.79
3:A:22:LYS:HD3	3:A:22:LYS:N	1.97	0.79
3:A:115:TYR:OH	3:A:157:PRO:HA	1.82	0.79
4:B:34:LEU:HD13	4:B:62:ALA:HB2	1.65	0.79
5:L:17:ASP:O	5:L:77:ASN:HA	1.83	0.79
3:A:138:GLU:HG2	3:A:139:THR:N	1.92	0.79
3:A:429:LEU:HD13	3:A:533:LEU:HD13	1.65	0.79
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.12	0.78
5:L:90:GLN:HE21	5:L:92:SER:H	1.31	0.78
5:L:120:PRO:CB	5:L:125:LEU:HD21	2.12	0.78
3:A:50:ILE:HG22	3:A:51:GLY:N	1.97	0.78
3:A:459:THR:HG22	3:A:463:ARG:HB3	1.63	0.78
6:H:133:PRO:O	6:H:134:LEU:HD23	1.83	0.78
6:H:166:SER:H	6:H:206:ASN:HD21	1.28	0.78
4:B:57:ASN:HD22	4:B:58:THR:N	1.82	0.78
4:B:242:GLN:HA	4:B:242:GLN:HE21	1.49	0.77
4:B:34:LEU:HD11	4:B:73:LYS:HG3	1.64	0.77
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.66	0.77
5:L:106:ILE:HG12	5:L:166:GLN:OE1	1.83	0.77
3:A:447:ASN:HD22	3:A:450:THR:HG23	1.50	0.77
3:A:498:ASP:HB2	3:A:538:ALA:HB2	1.65	0.77
3:A:23:GLN:HE22	3:A:60:VAL:H	1.34	0.76
3:A:209:LEU:HB3	3:A:214:LEU:HB2	1.67	0.76
3:A:437:ALA:HB1	3:A:493:VAL:HA	1.67	0.76
5:L:11:LEU:HD21	5:L:19:VAL:HG11	1.67	0.76
3:A:473:THR:O	3:A:476:LYS:N	2.18	0.76
3:A:450:THR:O	3:A:451:LYS:HG2	1.87	0.75
4:B:75:VAL:HG11	4:B:77:PHE:CZ	2.20	0.75
6:H:39:ILE:HG13	6:H:113:TRP:CH2	2.22	0.75
3:A:7:THR:HG22	3:A:119:PRO:HB2	1.68	0.74
6:H:148:LEU:HD13	6:H:220:ILE:HG21	1.69	0.74
3:A:5:ILE:HD11	3:A:167:ILE:HD11	1.70	0.74
3:A:320:ASP:H	3:A:343:GLN:HE22	1.35	0.74
3:A:469:LEU:HD21	3:A:480:GLN:HG2	1.68	0.74
3:A:215:THR:O	3:A:217:PRO:HD3	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:27:PHE:CE1	6:H:99:GLN:HG3	2.22	0.74
3:A:439:THR:HG21	4:B:289:LEU:N	2.01	0.74
6:H:69:LEU:CD2	6:H:84:MET:HE3	2.18	0.74
4:B:175:ASN:OD1	4:B:201:LYS:HE3	1.89	0.73
4:B:387:PRO:HG2	4:B:389:PHE:HE1	1.48	0.73
4:B:57:ASN:ND2	4:B:58:THR:N	2.35	0.73
3:A:90:VAL:HG12	4:B:141:GLY:H	1.52	0.73
4:B:423:VAL:C	4:B:425:LEU:H	1.96	0.73
3:A:138:GLU:CG	3:A:139:THR:H	1.95	0.72
4:B:146:TYR:CD2	4:B:150:PRO:HB3	2.23	0.72
4:B:296:THR:HG22	4:B:298:GLU:H	1.54	0.72
5:L:15:LEU:HD12	5:L:15:LEU:H	1.53	0.72
3:A:441:TYR:CD2	3:A:544:GLY:HA3	2.24	0.72
2:P:820:DC:H2''	2:P:821[A]:DC:H5'	1.71	0.72
3:A:478:GLU:OE1	3:A:498:ASP:CG	2.32	0.72
4:B:266:TRP:O	4:B:269:GLN:HG3	1.88	0.72
5:L:77:ASN:HD22	5:L:77:ASN:H	1.37	0.72
4:B:171:PHE:CE1	4:B:205:LEU:HA	2.25	0.72
5:L:89:GLN:HB2	5:L:98:PHE:CD1	2.25	0.72
4:B:377:THR:O	4:B:381:VAL:HG23	1.90	0.71
3:A:458:VAL:HG23	3:A:548:VAL:HG13	1.72	0.71
1:T:705:DA:C2	1:T:706:DT:C4	2.79	0.71
4:B:253:THR:O	4:B:257:ILE:HG12	1.90	0.71
5:L:61:ARG:CZ	5:L:79:GLU:HG3	2.19	0.71
5:L:46:LEU:HD23	5:L:55:HIS:CG	2.26	0.71
3:A:442:VAL:HB	3:A:481:ALA:HB1	1.73	0.71
3:A:473:THR:H	3:A:476:LYS:HG3	1.56	0.71
4:B:12:LEU:HD12	4:B:12:LEU:H	1.54	0.71
4:B:393:ILE:HD13	4:B:398:TRP:HB2	1.72	0.71
2:P:818:DC:H2'	2:P:819:DG:C8	2.24	0.70
3:A:337:TRP:CZ2	3:A:367:GLN:HB2	2.26	0.70
3:A:533:LEU:HD12	3:A:533:LEU:N	2.06	0.70
3:A:486:LEU:HD21	3:A:495:ILE:HD11	1.74	0.70
4:B:225:PRO:CB	4:B:226:PRO:HD3	2.17	0.70
4:B:340:GLN:HG3	4:B:351:THR:HG22	1.73	0.70
5:L:35:TRP:CZ3	5:L:88:CYS:HB3	2.27	0.70
4:B:47:ILE:HD12	4:B:146:TYR:HA	1.74	0.70
6:H:142:THR:C	6:H:144:SER:H	1.99	0.70
6:H:9:PRO:O	6:H:11:ILE:N	2.25	0.69
4:B:214:LEU:HD12	4:B:214:LEU:N	2.07	0.69
4:B:332:GLN:HA	4:B:332:GLN:OE1	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:373:GLN:NE2	4:B:397:THR:HG23	2.06	0.69
3:A:376:THR:CG2	3:A:386:THR:HG23	2.22	0.69
6:H:53:ILE:HB	6:H:71:VAL:CG1	2.21	0.69
3:A:454:LYS:HB2	3:A:454:LYS:HZ3	1.56	0.69
3:A:60:VAL:O	3:A:60:VAL:HG13	1.91	0.69
4:B:97:PRO:HB2	4:B:100:LEU:HB2	1.73	0.69
4:B:373:GLN:HE22	4:B:406:TRP:HA	1.58	0.69
5:L:136:LEU:HD22	5:L:175:MET:CE	2.22	0.69
3:A:257:ILE:HD11	3:A:293:ILE:HG21	1.74	0.69
4:B:225:PRO:HG3	5:L:92:SER:HA	1.75	0.69
3:A:30:LYS:O	3:A:33:ALA:HB3	1.93	0.68
4:B:363:ASN:O	4:B:367:GLN:HG3	1.93	0.68
3:A:420:PRO:HA	3:A:421:PRO:C	2.19	0.68
5:L:33:LEU:HD23	5:L:34:ASN:H	1.57	0.68
1:T:705:DA:C2	1:T:706:DT:C5	2.82	0.68
4:B:135:ILE:HD12	4:B:135:ILE:O	1.93	0.68
4:B:395:LYS:HB2	4:B:416:PHE:CD2	2.28	0.68
6:H:53:ILE:HD12	6:H:71:VAL:HG12	1.76	0.68
2:P:816:DG:H2'	2:P:817:MRG:H8	1.76	0.67
3:A:447:ASN:HB3	3:A:450:THR:OG1	1.94	0.67
4:B:225:PRO:HB2	4:B:226:PRO:CD	2.21	0.67
4:B:97:PRO:HD3	4:B:181:TYR:CD1	2.29	0.67
4:B:260:LEU:HD21	4:B:303:LEU:HD13	1.75	0.67
4:B:371:ALA:O	4:B:375:ILE:HG13	1.93	0.67
3:A:439:THR:CG2	4:B:288:ALA:HA	2.24	0.67
4:B:59:PRO:HG2	4:B:76:ASP:HB3	1.74	0.67
4:B:395:LYS:HB2	4:B:416:PHE:CE2	2.29	0.67
3:A:104:LYS:HB2	3:A:192:ASP:HA	1.75	0.67
4:B:31:ILE:O	4:B:35:VAL:HG23	1.94	0.67
4:B:100:LEU:HD22	4:B:381:VAL:HG13	1.77	0.67
4:B:329:ILE:HD11	4:B:375:ILE:HD12	1.76	0.67
3:A:454:LYS:HE2	3:A:554:ALA:HB3	1.77	0.67
4:B:2:ILE:HD12	4:B:3:SER:H	1.58	0.66
3:A:433:PRO:HD3	4:B:255:ASN:ND2	2.09	0.66
6:H:129:PRO:HB3	6:H:155:TYR:HB3	1.75	0.66
2:P:808:DC:H5'	2:P:808:DC:H6	1.61	0.66
3:A:106:VAL:HB	3:A:227:PHE:HE1	1.59	0.66
3:A:244:ILE:HG13	3:A:263:LYS:HD3	1.77	0.66
6:H:34:ILE:CG2	6:H:35:GLY:N	2.58	0.66
4:B:373:GLN:NE2	4:B:406:TRP:HA	2.11	0.66
3:A:25:PRO:O	3:A:26:LEU:HD23	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:12:LEU:HD12	4:B:12:LEU:N	2.10	0.65
3:A:440:PHE:HE2	3:A:489:SER:HG	1.44	0.65
2:P:817:MRG:H2'	2:P:818:DC:C6	2.32	0.65
3:A:434:ILE:HG22	3:A:494:ASN:ND2	2.10	0.65
4:B:244:ILE:H	4:B:244:ILE:CD1	2.08	0.65
3:A:371:ALA:O	3:A:375:ILE:HG12	1.96	0.65
6:H:183:ASP:O	6:H:184:LEU:HG	1.96	0.65
3:A:94:ILE:HD12	3:A:95:PRO:O	1.97	0.65
5:L:33:LEU:HD21	5:L:88:CYS:HB2	1.77	0.65
3:A:279:LEU:H	3:A:279:LEU:CD2	2.08	0.65
5:L:33:LEU:HD23	5:L:89:GLN:O	1.97	0.65
3:A:95:PRO:HD2	3:A:230:MET:HE2	1.80	0.64
3:A:442:VAL:HB	3:A:481:ALA:CB	2.28	0.64
3:A:149:LEU:HD11	3:A:159:ILE:HG22	1.78	0.64
3:A:458:VAL:HG12	3:A:458:VAL:O	1.97	0.64
3:A:473:THR:H	3:A:476:LYS:CG	2.10	0.64
4:B:225:PRO:HB3	5:L:32:TYR:CE1	2.32	0.64
5:L:50:TYR:O	5:L:52:SER:N	2.31	0.64
6:H:4:LEU:N	6:H:4:LEU:HD12	2.13	0.64
3:A:441:TYR:HD2	3:A:544:GLY:O	1.80	0.64
4:B:328:GLU:O	4:B:339:TYR:HA	1.98	0.64
5:L:90:GLN:HE21	5:L:92:SER:N	1.96	0.64
6:H:38:TRP:O	6:H:50:LEU:HB2	1.98	0.64
6:H:128:PRO:HA	6:H:209:HIS:HD2	1.63	0.64
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.33	0.63
3:A:529:GLU:O	3:A:530:LYS:HG3	1.99	0.63
3:A:548:VAL:O	3:A:552:VAL:HG23	1.98	0.63
4:B:237:ASP:C	4:B:239:TRP:N	2.56	0.63
4:B:116:PHE:HA	4:B:148:VAL:HG21	1.80	0.63
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.80	0.63
4:B:97:PRO:HG2	4:B:181:TYR:HB2	1.80	0.63
6:H:55:TRP:HE3	6:H:55:TRP:H	1.44	0.63
2:P:803:DC:H2''	2:P:804:DA:C8	2.33	0.63
5:L:120:PRO:O	5:L:125:LEU:HD11	1.98	0.63
4:B:79:GLU:OE1	4:B:83:ARG:NH1	2.31	0.63
5:L:90:GLN:NE2	5:L:92:SER:H	1.97	0.63
6:H:31:THR:OG1	6:H:34:ILE:HD13	1.97	0.63
3:A:27:THR:HG1	3:A:30:LYS:HG3	1.64	0.63
4:B:393:ILE:HG12	4:B:394:GLN:N	2.13	0.62
3:A:320:ASP:N	3:A:343:GLN:HE22	1.97	0.62
3:A:466:VAL:HG21	3:A:551:LEU:HG	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:144:ILE:HG12	5:L:145:ASN:H	1.63	0.62
3:A:465:LYS:HE3	3:A:488:ASP:OD2	2.00	0.62
3:A:507:GLN:O	3:A:509:GLN:HG2	1.99	0.62
5:L:115:VAL:HB	5:L:207:LYS:HG3	1.79	0.62
3:A:23:GLN:HG2	3:A:133:PRO:HD3	1.82	0.62
5:L:144:ILE:HG21	5:L:175:MET:CE	2.30	0.62
5:L:190:ASN:O	5:L:210:ASN:HA	1.99	0.62
6:H:39:ILE:HG23	6:H:48:GLU:O	2.00	0.62
4:B:239:TRP:CZ2	4:B:378:GLU:HG2	2.35	0.62
3:A:50:ILE:CG2	3:A:51:GLY:N	2.63	0.61
3:A:460:ASN:HA	4:B:286:THR:O	1.99	0.61
4:B:323:LYS:HB2	4:B:343:GLN:NE2	2.15	0.61
5:L:198:HIS:HD2	5:L:200:THR:HG23	1.64	0.61
3:A:478:GLU:OE1	3:A:498:ASP:OD2	2.19	0.61
5:L:175:MET:O	5:L:175:MET:HG2	2.00	0.61
6:H:62:ASN:ND2	6:H:64:SER:HB2	2.15	0.61
2:P:807:DC:H4'	3:A:448:ARG:HD2	1.81	0.61
3:A:430:GLU:HB2	3:A:532:TYR:HB2	1.83	0.61
4:B:131:THR:HG22	4:B:132:ILE:N	2.16	0.61
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.83	0.61
5:L:144:ILE:HG23	5:L:145:ASN:N	2.16	0.61
6:H:32:SER:O	6:H:55:TRP:CE2	2.54	0.61
6:H:209:HIS:CD2	6:H:212:SER:OG	2.54	0.61
3:A:445:ALA:O	3:A:477:THR:HG21	2.01	0.61
4:B:380:ILE:O	4:B:384:GLY:HA2	2.00	0.61
5:L:48:ILE:HG23	5:L:53:SER:O	2.00	0.61
3:A:279:LEU:HD23	3:A:279:LEU:N	2.15	0.61
5:L:61:ARG:CB	5:L:76:SER:HB3	2.22	0.61
1:T:705:DA:H2	1:T:706:DT:C7	2.14	0.60
4:B:47:ILE:HD11	4:B:146:TYR:CD1	2.36	0.60
5:L:118:PHE:CD2	6:H:134:LEU:HB3	2.36	0.60
5:L:46:LEU:HD23	5:L:55:HIS:ND1	2.15	0.60
3:A:337:TRP:HZ2	3:A:367:GLN:HB2	1.64	0.60
3:A:466:VAL:O	3:A:466:VAL:CG1	2.49	0.60
4:B:43:LYS:C	4:B:45:GLY:H	2.09	0.60
4:B:225:PRO:CG	5:L:92:SER:HA	2.31	0.60
5:L:63:SER:O	5:L:73:LEU:HD12	2.01	0.60
3:A:441:TYR:CE2	3:A:544:GLY:CA	2.84	0.60
3:A:538:ALA:HB1	3:A:539:HIS:HD2	1.66	0.60
6:H:152:VAL:HB	6:H:187:LEU:HD13	1.83	0.60
3:A:484:LEU:O	3:A:486:LEU:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:229:TRP:HA	4:B:232:TYR:CE1	2.37	0.60
5:L:19:VAL:O	5:L:74:THR:HA	2.02	0.60
5:L:144:ILE:CG2	5:L:175:MET:HE1	2.32	0.60
4:B:146:TYR:CE2	4:B:150:PRO:HA	2.37	0.60
4:B:330:GLN:HE22	4:B:340:GLN:NE2	2.00	0.60
4:B:230:MET:HE2	6:H:104:SER:HA	1.84	0.60
4:B:423:VAL:C	4:B:425:LEU:N	2.60	0.60
5:L:115:VAL:HG12	5:L:116:SER:N	2.17	0.60
3:A:495:ILE:HG22	3:A:496:VAL:N	2.16	0.60
3:A:246:LEU:H	3:A:246:LEU:CD2	2.06	0.59
3:A:501:TYR:CD1	3:A:505:ILE:HD11	2.35	0.59
5:L:34:ASN:OD1	5:L:49:TYR:CA	2.45	0.59
3:A:171:PHE:CE2	3:A:205:LEU:HD12	2.37	0.59
3:A:501:TYR:CZ	3:A:505:ILE:HD11	2.37	0.59
4:B:261:VAL:HG13	4:B:276:VAL:HG11	1.83	0.59
6:H:4:LEU:HD21	6:H:99:GLN:HB2	1.83	0.59
3:A:317:VAL:HG13	3:A:349:LEU:HD23	1.83	0.59
3:A:500:GLN:H	3:A:500:GLN:CD	2.10	0.59
4:B:149:LEU:HD13	4:B:156:SER:HA	1.84	0.59
6:H:92:THR:HG23	6:H:120:THR:CA	2.26	0.59
3:A:50:ILE:HD11	3:A:145:GLN:CB	2.05	0.59
3:A:363:ASN:HB2	3:A:511:ASP:HB3	1.84	0.59
4:B:210:LEU:C	4:B:212:TRP:H	2.08	0.59
3:A:181:TYR:HB2	3:A:188:TYR:HB3	1.82	0.59
3:A:257:ILE:O	3:A:261:VAL:HG12	2.02	0.59
3:A:517:LEU:O	3:A:521:ILE:HG13	2.03	0.59
4:B:299:ALA:C	4:B:301:LEU:N	2.59	0.59
3:A:5:ILE:CD1	3:A:167:ILE:HD11	2.32	0.59
3:A:9:PRO:HA	3:A:121:ASP:OD2	2.02	0.59
3:A:255:ASN:HB2	3:A:289:LEU:O	2.03	0.59
4:B:75:VAL:HG11	4:B:77:PHE:CE2	2.37	0.59
4:B:198:HIS:O	4:B:199:ARG:C	2.46	0.59
4:B:242:GLN:HA	4:B:242:GLN:NE2	2.18	0.59
4:B:368:LEU:O	4:B:372:VAL:HG23	2.03	0.59
5:L:18:ARG:HA	5:L:76:SER:O	2.02	0.59
6:H:162:VAL:HA	6:H:206:ASN:O	2.03	0.59
5:L:66:GLY:HA3	5:L:71:TYR:HA	1.85	0.58
3:A:215:THR:C	3:A:217:PRO:HD3	2.27	0.58
4:B:37:ILE:O	4:B:41:MET:HG3	2.01	0.58
6:H:40:ARG:HB2	6:H:50:LEU:HD11	1.85	0.58
4:B:360:ALA:HB1	4:B:367:GLN:HE21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:12:VAL:HG21	6:H:18:PHE:HB3	1.85	0.58
3:A:288:ALA:HB3	3:A:291:GLU:HB2	1.85	0.58
3:A:507:GLN:C	3:A:509:GLN:H	2.12	0.58
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.38	0.58
6:H:161:THR:HB	6:H:208:ALA:HB3	1.85	0.58
4:B:46:LYS:HD3	4:B:116:PHE:HB3	1.84	0.58
5:L:204:PRO:O	5:L:206:VAL:HG23	2.03	0.58
4:B:81:ASN:OD1	4:B:154:LYS:N	2.32	0.58
5:L:33:LEU:HD23	5:L:34:ASN:N	2.18	0.58
5:L:117:ILE:HD11	5:L:132:VAL:HG12	1.84	0.58
5:L:144:ILE:HG21	5:L:175:MET:HE2	1.86	0.58
5:L:148:TRP:CD2	5:L:179:LEU:HD13	2.38	0.58
5:L:159:VAL:HG22	5:L:179:LEU:HD12	1.85	0.58
3:A:493:VAL:HG22	3:A:494:ASN:N	2.17	0.58
4:B:69:THR:HG22	4:B:69:THR:O	2.04	0.58
3:A:471:ASN:O	3:A:472:THR:HG23	2.03	0.57
6:H:38:TRP:CZ3	6:H:97:CYS:HB3	2.39	0.57
3:A:531:VAL:HG12	3:A:532:TYR:N	2.19	0.57
4:B:12:LEU:HD21	4:B:127:TYR:CE1	2.38	0.57
4:B:162:SER:O	4:B:165:THR:HG22	2.04	0.57
5:L:77:ASN:HD22	5:L:77:ASN:N	2.00	0.57
6:H:134:LEU:HD12	6:H:149:GLY:HA3	1.85	0.57
3:A:443:ASP:CG	3:A:444:GLY:H	2.11	0.57
3:A:459:THR:HG21	3:A:463:ARG:HB3	1.86	0.57
5:L:4:MET:CE	5:L:90:GLN:HB2	2.31	0.57
5:L:11:LEU:CD2	5:L:19:VAL:HG11	2.32	0.57
5:L:19:VAL:HG12	5:L:20:THR:N	2.19	0.57
4:B:47:ILE:CD1	4:B:146:TYR:HA	2.35	0.57
4:B:299:ALA:C	4:B:301:LEU:H	2.11	0.57
2:P:808:DC:H5'	2:P:808:DC:C6	2.39	0.57
4:B:246:LEU:HD12	4:B:307:ARG:HB3	1.85	0.57
3:A:460:ASN:HA	4:B:286:THR:OG1	2.05	0.57
3:A:462:GLY:O	3:A:464:GLN:NE2	2.38	0.57
4:B:111:VAL:HG23	4:B:111:VAL:O	2.03	0.57
4:B:312:GLU:HB3	4:B:313:PRO:CD	2.34	0.57
4:B:325:LEU:HB3	4:B:387:PRO:HA	1.86	0.57
3:A:328:GLU:O	3:A:339:TYR:HA	2.05	0.56
4:B:118:VAL:O	4:B:148:VAL:HG23	2.05	0.56
5:L:77:ASN:H	5:L:77:ASN:ND2	2.02	0.56
5:L:162:SER:OG	6:H:177:PRO:HG2	2.05	0.56
3:A:368:LEU:O	3:A:372:VAL:HG23	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:258:GLN:O	4:B:259:LYS:C	2.48	0.56
3:A:76:ASP:OD1	3:A:78:ARG:HB2	2.05	0.56
3:A:408:ALA:O	3:A:409:THR:HG23	2.05	0.56
3:A:439:THR:HG21	4:B:288:ALA:HA	1.86	0.56
4:B:12:LEU:H	4:B:12:LEU:CD1	2.14	0.56
4:B:106:VAL:HG13	4:B:234:LEU:HB2	1.86	0.56
4:B:214:LEU:H	4:B:214:LEU:CD1	2.18	0.56
4:B:314:VAL:HG12	4:B:315:HIS:H	1.71	0.56
4:B:427:TYR:CE2	4:B:429:LEU:HB2	2.40	0.56
5:L:27:GLN:O	5:L:29:ILE:HG23	2.05	0.56
3:A:410:TRP:CZ2	3:A:412:PRO:HA	2.41	0.56
3:A:439:THR:O	3:A:441:TYR:CD1	2.59	0.56
3:A:503:LEU:CD2	3:A:535:TRP:HB2	2.35	0.56
4:B:214:LEU:HD12	4:B:214:LEU:H	1.70	0.56
5:L:120:PRO:HG3	5:L:131:SER:O	2.05	0.56
2:P:822[B]:TFO:C6'	3:A:184:MET:HG2	2.36	0.56
3:A:344:GLU:CB	3:A:345:PRO:HD2	2.35	0.56
4:B:247:PRO:HG3	4:B:427:TYR:OH	2.06	0.56
4:B:223:LYS:HD2	4:B:223:LYS:N	2.20	0.56
3:A:261:VAL:HA	3:A:264:LEU:HD12	1.88	0.56
6:H:209:HIS:CE1	6:H:211:ALA:HB3	2.40	0.56
3:A:506:ILE:O	3:A:510:PRO:HD2	2.05	0.56
4:B:104:LYS:HG2	4:B:192:ASP:HA	1.87	0.56
5:L:144:ILE:HG23	5:L:175:MET:HE1	1.88	0.56
5:L:170:ASP:O	5:L:172:THR:HG23	2.06	0.56
3:A:235:HIS:HB2	3:A:238:LYS:O	2.05	0.56
4:B:160:PHE:CE2	4:B:164:MET:HB2	2.40	0.56
4:B:260:LEU:HD12	4:B:260:LEU:O	2.06	0.56
5:L:79:GLU:HB3	5:L:80:PRO:HD2	1.87	0.56
2:P:822[B]:TFO:H8'1	3:A:185:ASP:OD1	2.04	0.55
3:A:233:GLU:HB2	3:A:240:THR:HG23	1.87	0.55
3:A:338:THR:HG22	3:A:339:TYR:N	2.20	0.55
5:L:90:GLN:HE22	5:L:93:LYS:H	1.53	0.55
6:H:59:ASN:ND2	6:H:59:ASN:H	2.04	0.55
3:A:22:LYS:H	3:A:22:LYS:CD	2.14	0.55
3:A:182:GLN:O	3:A:182:GLN:HG3	2.05	0.55
3:A:220:LYS:HE2	3:A:222:GLN:HB3	1.88	0.55
3:A:441:TYR:HD2	3:A:544:GLY:C	2.13	0.55
4:B:330:GLN:NE2	4:B:340:GLN:OE1	2.40	0.55
6:H:166:SER:N	6:H:206:ASN:ND2	2.53	0.55
3:A:317:VAL:HG22	3:A:318:TYR:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:89:GLN:HB2	5:L:98:PHE:CE1	2.42	0.55
3:A:439:THR:HA	3:A:494:ASN:HB2	1.88	0.55
4:B:47:ILE:HD11	4:B:146:TYR:CG	2.41	0.55
3:A:125:ARG:O	3:A:128:THR:N	2.35	0.55
5:L:86:TYR:O	5:L:101:GLY:HA2	2.06	0.55
5:L:28:ASP:HA	5:L:68:GLY:O	2.07	0.55
5:L:83:ILE:HD12	5:L:106:ILE:HG22	1.88	0.55
3:A:441:TYR:CD2	3:A:544:GLY:O	2.60	0.55
5:L:39:LYS:NZ	5:L:39:LYS:HB3	2.22	0.55
3:A:479:LEU:HD23	3:A:517:LEU:HD23	1.88	0.55
5:L:77:ASN:N	5:L:77:ASN:ND2	2.55	0.55
3:A:261:VAL:HG23	3:A:276:VAL:HG11	1.88	0.54
4:B:93:GLY:O	4:B:95:PRO:HD3	2.07	0.54
4:B:160:PHE:CD2	4:B:164:MET:HB2	2.42	0.54
4:B:279:LEU:HD11	4:B:302:GLU:CB	2.35	0.54
4:B:330:GLN:HE22	4:B:340:GLN:HE22	1.54	0.54
6:H:166:SER:H	6:H:206:ASN:ND2	2.02	0.54
2:P:808:DC:H2''	2:P:809:DC:O5'	2.05	0.54
3:A:86:ASP:HA	3:A:154:LYS:HZ2	1.72	0.54
4:B:106:VAL:HA	4:B:190:GLY:HA2	1.89	0.54
4:B:393:ILE:CG1	4:B:394:GLN:N	2.70	0.54
5:L:34:ASN:ND2	5:L:89:GLN:HE22	2.00	0.54
5:L:193:THR:HG23	5:L:208:SER:OG	2.08	0.54
6:H:142:THR:C	6:H:144:SER:N	2.66	0.54
4:B:31:ILE:O	4:B:32:LYS:C	2.50	0.54
4:B:262:GLY:O	4:B:265:ASN:HB3	2.07	0.54
6:H:10:GLY:HA2	6:H:118:SER:O	2.07	0.54
3:A:450:THR:HB	3:A:452:LEU:HG	1.90	0.54
3:A:479:LEU:HD21	3:A:518:VAL:CG2	2.38	0.54
4:B:214:LEU:N	4:B:214:LEU:CD1	2.70	0.54
4:B:314:VAL:HG12	4:B:315:HIS:N	2.22	0.54
5:L:107:LYS:HA	5:L:140:TYR:OH	2.07	0.54
5:L:150:ILE:HD12	5:L:155:ARG:HD3	1.88	0.54
1:T:713:DC:H2''	1:T:714:DG:H5'	1.90	0.54
6:H:34:ILE:HG23	6:H:35:GLY:N	2.22	0.54
3:A:21:VAL:HB	3:A:59:PRO:HD3	1.89	0.54
5:L:34:ASN:ND2	6:H:109:ALA:HB2	2.22	0.54
6:H:152:VAL:HB	6:H:187:LEU:CD1	2.38	0.54
4:B:329:ILE:O	4:B:392:PRO:HG3	2.08	0.54
5:L:34:ASN:O	5:L:88:CYS:HA	2.08	0.54
6:H:59:ASN:O	6:H:60:ARG:HD3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:273:GLY:O	3:A:274:ILE:HD13	2.08	0.53
3:A:425:LEU:HD13	3:A:509:GLN:OE1	2.07	0.53
4:B:363:ASN:C	4:B:363:ASN:HD22	2.16	0.53
3:A:503:LEU:C	3:A:503:LEU:HD12	2.33	0.53
3:A:41:MET:HE1	3:A:73:LYS:CE	2.38	0.53
6:H:162:VAL:HG22	6:H:207:VAL:HG22	1.90	0.53
6:H:169:LEU:HD23	6:H:191:VAL:HG21	1.90	0.53
4:B:43:LYS:C	4:B:45:GLY:N	2.65	0.53
4:B:116:PHE:C	4:B:148:VAL:HG21	2.33	0.53
1:T:705:DA:C2	1:T:706:DT:H72	2.36	0.53
1:T:706:DT:O2	1:T:707:DG:N7	2.42	0.53
1:T:709:DC:H2''	1:T:710:DG:H5'	1.91	0.53
3:A:397:THR:HG21	3:A:424:LYS:HA	1.90	0.53
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.89	0.53
4:B:77:PHE:O	4:B:81:ASN:ND2	2.41	0.53
4:B:223:LYS:HE3	6:H:58:ASP:HB3	1.90	0.53
4:B:292:VAL:C	4:B:293:ILE:HD13	2.32	0.53
5:L:6:GLN:OE1	5:L:101:GLY:N	2.42	0.53
6:H:150:CYS:HB2	6:H:164:TRP:CH2	2.43	0.53
5:L:90:GLN:NE2	5:L:92:SER:N	2.56	0.53
6:H:9:PRO:C	6:H:11:ILE:H	2.15	0.53
2:P:822[B]:TFO:H6'2	3:A:184:MET:HG2	1.91	0.53
4:B:423:VAL:O	4:B:425:LEU:N	2.36	0.53
5:L:88:CYS:O	5:L:98:PHE:HA	2.08	0.53
2:P:816:DG:H2'	2:P:817:MRG:C8	2.38	0.53
3:A:340:GLN:HB3	3:A:348:ASN:OD1	2.08	0.53
3:A:440:PHE:HE2	3:A:489:SER:OG	1.92	0.53
3:A:454:LYS:HA	3:A:469:LEU:HD12	1.91	0.53
3:A:486:LEU:HA	3:A:528:LYS:NZ	2.24	0.53
4:B:108:VAL:HG12	4:B:188:TYR:CE1	2.44	0.53
3:A:363:ASN:OD1	3:A:364:ASP:N	2.42	0.52
4:B:110:ASP:HB3	4:B:217:PRO:HG2	1.92	0.52
5:L:90:GLN:CD	5:L:90:GLN:C	2.76	0.52
6:H:69:LEU:HD22	6:H:82:LEU:HD11	1.91	0.52
3:A:18:GLY:HA3	3:A:56:TYR:CD2	2.44	0.52
3:A:171:PHE:CZ	3:A:205:LEU:HD12	2.44	0.52
3:A:503:LEU:HD12	3:A:503:LEU:O	2.09	0.52
5:L:2:ILE:HD12	5:L:90:GLN:CD	2.34	0.52
5:L:89:GLN:HA	5:L:97:THR:O	2.08	0.52
1:T:724:DT:H2''	1:T:725:DG:C8	2.45	0.52
5:L:151:ASP:C	5:L:153:SER:H	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:705:DA:C2	1:T:706:DT:C7	2.92	0.52
4:B:56:TYR:N	4:B:56:TYR:CD1	2.78	0.52
4:B:58:THR:HG23	4:B:59:PRO:HD2	1.91	0.52
4:B:181:TYR:HB3	4:B:188:TYR:HB2	1.92	0.52
4:B:224:GLU:HB3	4:B:225:PRO:HD2	1.92	0.52
4:B:262:GLY:O	4:B:265:ASN:N	2.42	0.52
3:A:295:LEU:HD23	3:A:300:GLU:CD	2.35	0.52
5:L:90:GLN:CD	5:L:90:GLN:O	2.53	0.52
5:L:144:ILE:CG2	5:L:175:MET:CE	2.88	0.52
3:A:90:VAL:CG1	4:B:141:GLY:H	2.20	0.52
3:A:532:TYR:C	3:A:532:TYR:CD2	2.87	0.52
1:T:716:DA:H1'	1:T:717:DC:H5'	1.92	0.52
2:P:822[A]:TFO:C2	3:A:219:LYS:HD3	2.40	0.52
3:A:220:LYS:O	3:A:220:LYS:HD3	2.08	0.52
3:A:465:LYS:O	3:A:466:VAL:CG2	2.56	0.52
4:B:304:ALA:HA	4:B:307:ARG:HG2	1.92	0.52
3:A:494:ASN:OD1	4:B:289:LEU:HD12	2.09	0.52
4:B:170:PRO:HB2	4:B:208:HIS:HE1	1.73	0.52
4:B:299:ALA:O	4:B:301:LEU:N	2.43	0.52
3:A:439:THR:O	3:A:439:THR:OG1	2.28	0.51
5:L:20:THR:HA	5:L:73:LEU:O	2.10	0.51
3:A:254:VAL:HG13	3:A:255:ASN:N	2.24	0.51
3:A:439:THR:HG23	4:B:288:ALA:HA	1.92	0.51
4:B:115:TYR:C	4:B:117:SER:H	2.18	0.51
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.45	0.51
6:H:39:ILE:HD11	6:H:110:MET:SD	2.51	0.51
3:A:331:LYS:HD3	3:A:332:GLN:N	2.25	0.51
4:B:7:THR:OG1	4:B:121:ASP:HA	2.11	0.51
4:B:258:GLN:O	4:B:261:VAL:N	2.43	0.51
3:A:13:LYS:HB2	3:A:16:MET:HE3	1.91	0.51
3:A:376:THR:HG23	3:A:386:THR:HG23	1.92	0.51
3:A:511:ASP:OD2	3:A:511:ASP:C	2.52	0.51
6:H:16:GLN:O	6:H:87:VAL:HG22	2.10	0.51
4:B:107:THR:HG22	4:B:108:VAL:N	2.26	0.51
4:B:171:PHE:HE1	4:B:205:LEU:HA	1.70	0.51
6:H:95:TYR:O	6:H:116:GLY:HA2	2.11	0.51
3:A:13:LYS:CB	3:A:16:MET:HE3	2.41	0.51
3:A:38:CYS:HA	3:A:41:MET:HE3	1.92	0.51
3:A:115:TYR:C	3:A:117:SER:H	2.19	0.51
3:A:258:CYS:HA	3:A:261:VAL:CG1	2.41	0.51
3:A:406:TRP:CZ2	4:B:420:PRO:HG3	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:10:VAL:HG22	4:B:87:PHE:CE1	2.46	0.51
4:B:34:LEU:CD1	4:B:73:LYS:HG3	2.38	0.51
4:B:330:GLN:HE22	4:B:340:GLN:CD	2.17	0.51
5:L:31:SER:HA	5:L:71:TYR:HE2	1.76	0.51
5:L:34:ASN:HD21	6:H:109:ALA:HB2	1.73	0.51
6:H:57:ASP:OD2	6:H:73:LYS:HE2	2.11	0.51
3:A:50:ILE:CG1	3:A:145:GLN:HB2	2.40	0.51
3:A:504:GLY:O	3:A:505:ILE:C	2.53	0.51
4:B:100:LEU:HD23	4:B:100:LEU:O	2.11	0.51
2:P:806:DT:C2	2:P:807:DC:C5	2.99	0.51
3:A:96:HIS:CG	3:A:97:PRO:HD2	2.46	0.51
3:A:539:HIS:N	3:A:539:HIS:CD2	2.79	0.51
4:B:28:GLU:O	4:B:31:ILE:N	2.44	0.51
4:B:153:TRP:O	4:B:155:GLY:N	2.44	0.51
4:B:163:SER:O	4:B:167:ILE:HG13	2.11	0.51
1:T:711:DC:H2'	1:T:712:DC:C6	2.46	0.51
3:A:441:TYR:CD2	3:A:544:GLY:C	2.89	0.51
3:A:473:THR:O	3:A:474:ASN:C	2.53	0.51
4:B:252:TRP:HB2	4:B:257:ILE:HD11	1.93	0.51
3:A:443:ASP:OD1	3:A:478:GLU:OE1	2.29	0.50
4:B:295:LEU:HD22	4:B:300:GLU:N	2.26	0.50
4:B:29:GLU:HG2	4:B:71:TRP:CZ2	2.47	0.50
4:B:124:PHE:CG	4:B:124:PHE:O	2.64	0.50
3:A:484:LEU:O	3:A:487:GLN:N	2.45	0.50
4:B:23:GLN:OE1	4:B:59:PRO:HA	2.11	0.50
4:B:106:VAL:HG13	4:B:234:LEU:CB	2.41	0.50
5:L:90:GLN:NE2	5:L:93:LYS:H	2.08	0.50
2:P:822[B]:TFO:H8	2:P:822[B]:TFO:OP1	2.11	0.50
3:A:3:SER:HB3	3:A:5:ILE:CG1	2.36	0.50
3:A:143:ARG:HG3	3:A:143:ARG:HH11	1.77	0.50
3:A:439:THR:O	3:A:441:TYR:CE1	2.63	0.50
3:A:451:LYS:O	3:A:471:ASN:N	2.44	0.50
3:A:473:THR:O	3:A:475:GLN:N	2.43	0.50
4:B:227:PHE:HD1	6:H:104:SER:O	1.95	0.50
3:A:128:THR:CB	3:A:146:TYR:HB2	2.42	0.50
3:A:188:TYR:HE2	3:A:234:LEU:HD13	1.75	0.50
3:A:380:ILE:O	3:A:384:GLY:HA2	2.12	0.50
3:A:489:SER:HB3	3:A:528:LYS:HZ3	1.77	0.50
3:A:507:GLN:C	3:A:509:GLN:N	2.70	0.50
4:B:131:THR:CG2	4:B:132:ILE:N	2.75	0.50
4:B:372:VAL:HG13	4:B:389:PHE:CD2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:148:LEU:HD13	6:H:220:ILE:CG2	2.40	0.50
6:H:174:HIS:O	6:H:189:SER:HA	2.11	0.50
1:T:706:DT:O2	1:T:706:DT:C2'	2.60	0.50
3:A:479:LEU:HD21	3:A:518:VAL:HG22	1.94	0.50
3:A:486:LEU:HD21	3:A:495:ILE:CD1	2.41	0.50
3:A:261:VAL:O	3:A:264:LEU:HB2	2.11	0.50
3:A:325:LEU:HD12	3:A:343:GLN:HG2	1.93	0.50
4:B:28:GLU:O	4:B:29:GLU:C	2.54	0.50
3:A:154:LYS:O	3:A:157:PRO:HD2	2.12	0.50
3:A:353:LYS:HD2	3:A:353:LYS:O	2.11	0.50
3:A:441:TYR:CD2	3:A:544:GLY:CA	2.93	0.50
3:A:542:ILE:O	3:A:543:GLY:O	2.29	0.50
3:A:132:ILE:CG2	3:A:142:ILE:HB	2.41	0.49
3:A:361:HIS:CD2	3:A:505:ILE:HG23	2.47	0.49
3:A:484:LEU:C	3:A:486:LEU:N	2.70	0.49
4:B:7:THR:HG23	4:B:7:THR:O	2.12	0.49
4:B:227:PHE:HB2	6:H:105:VAL:HA	1.93	0.49
4:B:378:GLU:O	4:B:382:ILE:HG13	2.12	0.49
3:A:138:GLU:OE1	3:A:139:THR:HG22	2.11	0.49
3:A:538:ALA:CB	3:A:539:HIS:HD2	2.25	0.49
4:B:37:ILE:HD13	4:B:73:LYS:HB2	1.94	0.49
1:T:709:DC:H2'	1:T:710:DG:H8	1.76	0.49
4:B:101:LYS:O	4:B:236:PRO:HB2	2.12	0.49
4:B:261:VAL:HG13	4:B:276:VAL:CG1	2.42	0.49
3:A:401:TRP:CZ2	3:A:405:TYR:CD2	3.00	0.49
5:L:117:ILE:HD12	5:L:134:CYS:HB2	1.93	0.49
3:A:125:ARG:HB3	3:A:145:GLN:CG	2.42	0.49
3:A:439:THR:OG1	3:A:441:TYR:HE1	1.96	0.49
5:L:49:TYR:CD2	5:L:49:TYR:N	2.80	0.49
3:A:160:PHE:C	3:A:160:PHE:CD2	2.89	0.49
3:A:292:VAL:HG12	3:A:293:ILE:N	2.28	0.49
6:H:147:THR:HG23	6:H:192:THR:OG1	2.12	0.49
1:T:707:DG:H2''	1:T:708:DG:H5'	1.93	0.49
3:A:411:ILE:CG2	3:A:412:PRO:HD2	2.42	0.49
3:A:500:GLN:NE2	3:A:500:GLN:N	2.55	0.49
4:B:75:VAL:CG1	4:B:77:PHE:CE2	2.96	0.49
3:A:186:ASP:O	3:A:187:LEU:HD23	2.12	0.49
3:A:320:ASP:H	3:A:343:GLN:NE2	2.06	0.49
4:B:210:LEU:C	4:B:212:TRP:N	2.70	0.49
6:H:24:PHE:CE1	6:H:78:ASN:HB3	2.48	0.49
1:T:706:DT:H72	3:A:151:GLN:HG3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:493:VAL:CG2	3:A:494:ASN:N	2.75	0.49
4:B:67:ASP:OD2	4:B:219:LYS:HG2	2.12	0.49
5:L:117:ILE:HG13	5:L:118:PHE:N	2.28	0.49
5:L:182:THR:HG22	5:L:183:LYS:H	1.78	0.49
5:L:190:ASN:HD22	5:L:211:ARG:HG2	1.77	0.49
3:A:69:THR:O	3:A:69:THR:HG22	2.13	0.49
4:B:13:LYS:HE2	4:B:85:GLN:HB3	1.95	0.49
4:B:327:ALA:HA	4:B:340:GLN:O	2.13	0.49
6:H:27:PHE:CZ	6:H:99:GLN:HG3	2.47	0.49
4:B:60:VAL:HG12	4:B:75:VAL:HA	1.95	0.48
3:A:484:LEU:C	3:A:486:LEU:H	2.21	0.48
4:B:108:VAL:CG1	4:B:188:TYR:CE1	2.96	0.48
1:T:708:DG:OP1	3:A:89:GLU:HG3	2.14	0.48
3:A:60:VAL:O	3:A:60:VAL:CG1	2.61	0.48
3:A:227:PHE:HB2	3:A:234:LEU:HB2	1.95	0.48
3:A:394:GLN:O	3:A:395:LYS:C	2.55	0.48
5:L:83:ILE:CG2	5:L:106:ILE:HG23	2.34	0.48
5:L:147:LYS:HE2	5:L:149:LYS:HD2	1.95	0.48
3:A:50:ILE:HG22	3:A:51:GLY:H	1.74	0.48
3:A:257:ILE:HB	3:A:283:LEU:HD21	1.96	0.48
3:A:536:VAL:HG13	3:A:537:PRO:HD2	1.94	0.48
4:B:329:ILE:HA	4:B:338:THR:O	2.14	0.48
3:A:31:ILE:C	3:A:33:ALA:N	2.70	0.48
3:A:459:THR:HG22	3:A:463:ARG:CB	2.41	0.48
6:H:39:ILE:HG13	6:H:113:TRP:CZ3	2.49	0.48
6:H:142:THR:O	6:H:144:SER:N	2.47	0.48
4:B:231:GLY:O	4:B:233:GLU:O	2.32	0.48
4:B:264:LEU:HD22	4:B:306:ASN:ND2	2.29	0.48
5:L:191:SER:HB2	5:L:210:ASN:HD21	1.79	0.48
6:H:18:PHE:CD2	6:H:87:VAL:HG11	2.49	0.48
6:H:32:SER:O	6:H:55:TRP:CD2	2.67	0.48
3:A:274:ILE:HD13	3:A:309:ILE:HD12	1.95	0.48
4:B:193:LEU:HD12	4:B:198:HIS:N	2.29	0.48
4:B:420:PRO:HB3	4:B:421:PRO:HD2	1.96	0.48
1:T:712:DC:H2'	1:T:713:DC:H6	1.77	0.48
3:A:128:THR:OG1	3:A:146:TYR:HB2	2.14	0.48
3:A:498:ASP:OD1	3:A:498:ASP:N	2.45	0.48
3:A:507:GLN:O	3:A:509:GLN:N	2.47	0.48
3:A:509:GLN:N	3:A:510:PRO:CD	2.77	0.48
4:B:372:VAL:HG13	4:B:389:PHE:CE2	2.49	0.48
5:L:17:ASP:HB2	5:L:78:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:173:TYR:N	5:L:173:TYR:CD1	2.81	0.48
3:A:254:VAL:HA	3:A:257:ILE:HD12	1.95	0.48
6:H:82:LEU:HD12	6:H:83:ASN:N	2.28	0.48
6:H:97:CYS:O	6:H:97:CYS:SG	2.72	0.48
1:T:706:DT:O2	1:T:706:DT:H2'	2.13	0.47
4:B:112:GLY:HA3	4:B:151:GLN:HE21	1.79	0.47
4:B:221:HIS:HB3	4:B:229:TRP:CD1	2.48	0.47
5:L:151:ASP:O	5:L:153:SER:N	2.44	0.47
3:A:244:ILE:O	3:A:244:ILE:HG23	2.14	0.47
3:A:410:TRP:CG	3:A:411:ILE:N	2.83	0.47
4:B:410:TRP:C	4:B:410:TRP:HE3	2.21	0.47
1:T:705:DA:N1	1:T:706:DT:O4	2.48	0.47
3:A:342:TYR:CD1	3:A:342:TYR:N	2.82	0.47
3:A:456:GLY:O	3:A:548:VAL:HG12	2.14	0.47
3:A:476:LYS:O	3:A:479:LEU:HB3	2.14	0.47
3:A:494:ASN:HB3	4:B:289:LEU:HD12	1.95	0.47
4:B:97:PRO:O	4:B:98:ALA:C	2.57	0.47
6:H:59:ASN:ND2	6:H:59:ASN:N	2.60	0.47
3:A:477:THR:O	3:A:480:GLN:N	2.47	0.47
5:L:46:LEU:HB3	5:L:55:HIS:ND1	2.30	0.47
6:H:40:ARG:HD3	6:H:50:LEU:HD11	1.96	0.47
6:H:56:ASP:OD2	6:H:58:ASP:CB	2.62	0.47
5:L:70:ASP:C	5:L:71:TYR:CD1	2.92	0.47
3:A:366:LYS:O	3:A:369:THR:HB	2.15	0.47
3:A:480:GLN:NE2	3:A:517:LEU:HD11	2.29	0.47
3:A:556:ILE:HG12	3:A:556:ILE:O	2.13	0.47
5:L:120:PRO:HB3	5:L:125:LEU:HD21	1.95	0.47
5:L:180:THR:C	5:L:181:LEU:HD12	2.40	0.47
3:A:400:THR:O	3:A:403:THR:HG22	2.14	0.47
4:B:76:ASP:OD1	4:B:78:ARG:NE	2.47	0.47
4:B:314:VAL:HB	4:B:317:VAL:CG2	2.44	0.47
5:L:35:TRP:HB2	5:L:48:ILE:HD12	1.96	0.47
5:L:36:TYR:CE1	5:L:46:LEU:HD12	2.49	0.47
5:L:120:PRO:O	5:L:125:LEU:CD1	2.63	0.47
6:H:142:THR:CG2	6:H:144:SER:OG	2.63	0.47
4:B:104:LYS:CG	4:B:192:ASP:HA	2.45	0.47
4:B:260:LEU:HD11	4:B:264:LEU:CD1	2.45	0.47
3:A:419:THR:HG23	3:A:419:THR:O	2.15	0.47
3:A:441:TYR:O	3:A:548:VAL:HG11	2.15	0.47
4:B:1:PRO:O	4:B:3:SER:N	2.48	0.47
4:B:27:THR:O	4:B:28:GLU:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:286:THR:O	4:B:286:THR:OG1	2.31	0.47
5:L:81:GLU:OE1	5:L:81:GLU:N	2.47	0.47
4:B:254:VAL:HG21	4:B:288:ALA:O	2.15	0.47
4:B:302:GLU:OE1	4:B:302:GLU:HA	2.15	0.47
5:L:33:LEU:CD2	5:L:88:CYS:HB2	2.44	0.47
5:L:125:LEU:HD23	5:L:129:GLY:O	2.15	0.47
5:L:170:ASP:C	5:L:170:ASP:OD1	2.58	0.47
6:H:34:ILE:HG23	6:H:35:GLY:H	1.80	0.47
6:H:142:THR:HG21	6:H:144:SER:OG	2.15	0.47
3:A:338:THR:HG22	3:A:340:GLN:NE2	2.29	0.46
3:A:486:LEU:CD2	3:A:495:ILE:HD11	2.43	0.46
6:H:125:LYS:O	6:H:126:THR:C	2.58	0.46
3:A:342:TYR:N	3:A:342:TYR:HD1	2.13	0.46
3:A:493:VAL:C	3:A:494:ASN:HD22	2.24	0.46
4:B:116:PHE:CA	4:B:148:VAL:HG21	2.45	0.46
4:B:242:GLN:HE21	4:B:242:GLN:CA	2.15	0.46
3:A:442:VAL:CB	3:A:481:ALA:HB1	2.44	0.46
4:B:394:GLN:O	4:B:395:LYS:C	2.57	0.46
5:L:2:ILE:HD11	5:L:93:LYS:HB3	1.96	0.46
6:H:148:LEU:HD12	6:H:203:VAL:HG11	1.97	0.46
3:A:18:GLY:HA3	3:A:56:TYR:CE2	2.51	0.46
3:A:442:VAL:HG21	3:A:482:ILE:HG12	1.96	0.46
3:A:511:ASP:O	3:A:511:ASP:CG	2.58	0.46
4:B:85:GLN:O	4:B:85:GLN:HG2	2.16	0.46
4:B:200:THR:HG22	4:B:201:LYS:N	2.29	0.46
4:B:222:GLN:HE21	4:B:224:GLU:CG	2.20	0.46
5:L:73:LEU:HD12	5:L:74:THR:H	1.79	0.46
5:L:120:PRO:O	5:L:121:SER:C	2.59	0.46
6:H:155:TYR:CE1	6:H:160:VAL:HG13	2.50	0.46
2:P:808:DC:H1'	2:P:809:DC:H5'	1.96	0.46
3:A:209:LEU:HB3	3:A:214:LEU:CB	2.40	0.46
3:A:411:ILE:HG23	3:A:412:PRO:HD2	1.98	0.46
3:A:543:GLY:C	3:A:545:ASN:H	2.24	0.46
4:B:113:ASP:C	4:B:115:TYR:N	2.73	0.46
5:L:60:SER:C	5:L:62:PHE:H	2.22	0.46
3:A:482:ILE:HD11	3:A:497:THR:HG21	1.97	0.46
4:B:146:TYR:CG	4:B:150:PRO:HB3	2.51	0.46
4:B:100:LEU:HD11	4:B:188:TYR:HB3	1.98	0.46
1:T:706:DT:H73	3:A:115:TYR:CE2	2.51	0.46
3:A:261:VAL:HG13	3:A:262:GLY:N	2.31	0.46
3:A:280:SER:C	3:A:282:LEU:H	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:489:SER:HB3	3:A:528:LYS:NZ	2.31	0.46
4:B:43:LYS:O	4:B:45:GLY:N	2.49	0.46
4:B:107:THR:HG22	4:B:108:VAL:H	1.81	0.46
4:B:231:GLY:O	4:B:232:TYR:C	2.59	0.46
4:B:254:VAL:O	4:B:255:ASN:C	2.58	0.46
5:L:83:ILE:HD12	5:L:106:ILE:CG2	2.46	0.46
6:H:18:PHE:HD2	6:H:87:VAL:HG11	1.81	0.46
2:P:815:DG:H2'	2:P:816:DG:C8	2.51	0.46
3:A:50:ILE:CG2	3:A:51:GLY:H	2.27	0.46
3:A:362:THR:OG1	3:A:363:ASN:N	2.47	0.46
3:A:440:PHE:CZ	3:A:488:ASP:O	2.69	0.46
5:L:121:SER:O	5:L:122:SER:C	2.58	0.46
3:A:391:LEU:HA	3:A:392:PRO:HD3	1.79	0.45
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.73	0.45
4:B:47:ILE:HD12	4:B:47:ILE:HA	1.68	0.45
4:B:153:TRP:CZ3	4:B:155:GLY:HA3	2.50	0.45
5:L:146:VAL:CG1	5:L:147:LYS:N	2.77	0.45
5:L:198:HIS:C	5:L:200:THR:H	2.24	0.45
1:T:712:DC:H2'	1:T:713:DC:C6	2.51	0.45
3:A:3:SER:HA	3:A:4:PRO:HD3	1.71	0.45
3:A:56:TYR:O	3:A:143:ARG:NH2	2.49	0.45
3:A:261:VAL:HG13	3:A:262:GLY:H	1.81	0.45
4:B:29:GLU:HG2	4:B:71:TRP:CH2	2.50	0.45
5:L:198:HIS:CD2	5:L:200:THR:HG23	2.49	0.45
6:H:54:TRP:CE3	6:H:55:TRP:HZ3	2.33	0.45
3:A:414:TRP:CE3	3:A:415:GLU:O	2.70	0.45
4:B:207:GLN:O	4:B:208:HIS:C	2.59	0.45
5:L:117:ILE:C	5:L:118:PHE:CD1	2.94	0.45
6:H:6:GLU:HB3	6:H:117:THR:OG1	2.16	0.45
6:H:156:PHE:HA	6:H:157:PRO:HA	1.72	0.45
1:T:705:DA:H5'	1:T:705:DA:H8	1.81	0.45
3:A:376:THR:O	3:A:377:THR:C	2.59	0.45
3:A:401:TRP:HE3	3:A:401:TRP:HA	1.81	0.45
3:A:457:TYR:C	3:A:458:VAL:HG23	2.42	0.45
4:B:263:LYS:O	4:B:264:LEU:C	2.59	0.45
4:B:271:TYR:O	4:B:274:ILE:HG12	2.16	0.45
4:B:281:LYS:C	4:B:283:LEU:N	2.74	0.45
5:L:31:SER:HA	5:L:71:TYR:CE2	2.50	0.45
5:L:50:TYR:C	5:L:52:SER:H	2.23	0.45
1:T:716:DA:C2	1:T:717:DC:C2	3.05	0.45
1:T:724:DT:H2''	1:T:725:DG:H8	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:LEU:O	3:A:13:LYS:C	2.59	0.45
3:A:344:GLU:HG3	3:A:345:PRO:CD	2.26	0.45
3:A:364:ASP:HB3	3:A:423:VAL:HG13	1.97	0.45
3:A:401:TRP:HA	3:A:401:TRP:CE3	2.52	0.45
3:A:463:ARG:HG3	3:A:464:GLN:N	2.32	0.45
3:A:531:VAL:HG12	3:A:532:TYR:H	1.81	0.45
4:B:156:SER:N	4:B:157:PRO:HD2	2.32	0.45
5:L:94:PHE:HA	5:L:95:PRO:C	2.41	0.45
3:A:203:GLU:HG3	3:A:207:GLN:HE21	1.81	0.45
3:A:272:PRO:O	3:A:273:GLY:O	2.34	0.45
4:B:263:LYS:HE2	4:B:424:LYS:HB2	1.97	0.45
5:L:108:ARG:HH11	5:L:108:ARG:HG3	1.81	0.45
5:L:132:VAL:O	5:L:148:TRP:CH2	2.70	0.45
2:P:822[B]:TFO:H6'1	3:A:184:MET:HG2	1.98	0.45
3:A:111:VAL:HG21	3:A:164:MET:HE1	1.97	0.45
3:A:171:PHE:CE1	3:A:205:LEU:HB2	2.50	0.45
4:B:239:TRP:CH2	4:B:378:GLU:HA	2.52	0.45
5:L:109:ALA:O	5:L:110:ASP:O	2.35	0.45
5:L:172:THR:C	5:L:173:TYR:CD1	2.95	0.45
6:H:54:TRP:HB3	6:H:55:TRP:CE3	2.52	0.45
3:A:439:THR:HG21	4:B:288:ALA:CA	2.47	0.45
4:B:156:SER:O	4:B:157:PRO:C	2.59	0.45
4:B:160:PHE:O	4:B:161:GLN:C	2.59	0.45
4:B:195:ILE:HG12	4:B:199:ARG:HD3	1.98	0.45
3:A:457:TYR:O	3:A:458:VAL:HG23	2.17	0.45
4:B:276:VAL:O	4:B:280:SER:N	2.50	0.45
4:B:417:VAL:O	4:B:417:VAL:HG23	2.16	0.45
6:H:40:ARG:HB2	6:H:50:LEU:CD1	2.47	0.45
6:H:198:TRP:CH2	6:H:222:PRO:HB3	2.52	0.45
3:A:465:LYS:HG3	3:A:466:VAL:N	2.30	0.45
3:A:482:ILE:O	3:A:486:LEU:HG	2.17	0.45
4:B:55:PRO:HG2	4:B:56:TYR:CE1	2.52	0.45
4:B:221:HIS:HB3	4:B:229:TRP:CG	2.51	0.45
4:B:324:ASP:O	4:B:343:GLN:HG2	2.17	0.45
5:L:83:ILE:HG22	5:L:104:LEU:O	2.17	0.45
5:L:132:VAL:O	5:L:148:TRP:HH2	1.99	0.45
1:T:706:DT:H2"	1:T:707:DG:H8	1.82	0.44
3:A:34:LEU:O	3:A:37:ILE:HG13	2.18	0.44
4:B:123:ASP:C	4:B:125:ARG:H	2.26	0.44
4:B:206:ARG:NH1	4:B:217:PRO:O	2.50	0.44
4:B:252:TRP:CD1	4:B:252:TRP:N	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:48:ILE:CG2	5:L:53:SER:O	2.64	0.44
6:H:133:PRO:C	6:H:134:LEU:HD23	2.42	0.44
3:A:198:HIS:O	3:A:201:LYS:N	2.45	0.44
3:A:220:LYS:HD3	3:A:220:LYS:C	2.42	0.44
6:H:126:THR:HA	6:H:156:PHE:O	2.17	0.44
3:A:41:MET:HE1	3:A:73:LYS:NZ	2.32	0.44
3:A:454:LYS:CE	3:A:554:ALA:HB3	2.46	0.44
5:L:146:VAL:HG12	5:L:147:LYS:N	2.31	0.44
3:A:166:LYS:NZ	3:A:166:LYS:HB3	2.33	0.44
3:A:368:LEU:O	3:A:369:THR:C	2.58	0.44
6:H:89:THR:HA	6:H:121:VAL:HB	1.99	0.44
3:A:50:ILE:CG1	3:A:145:GLN:CB	2.95	0.44
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.52	0.44
6:H:105:VAL:HG12	6:H:105:VAL:O	2.16	0.44
6:H:155:TYR:O	6:H:185:TYR:HB2	2.17	0.44
3:A:109:LEU:HD23	3:A:220:LYS:HB2	2.00	0.44
4:B:18:GLY:HA3	4:B:56:TYR:CD2	2.52	0.44
4:B:170:PRO:HB2	4:B:208:HIS:CE1	2.51	0.44
3:A:23:GLN:HE22	3:A:60:VAL:N	2.10	0.44
3:A:132:ILE:HG23	3:A:132:ILE:O	2.18	0.44
3:A:376:THR:O	3:A:379:SER:N	2.43	0.44
3:A:414:TRP:HE3	3:A:415:GLU:O	2.01	0.44
4:B:225:PRO:CB	4:B:226:PRO:CD	2.85	0.44
4:B:395:LYS:CB	4:B:416:PHE:CE2	3.00	0.44
6:H:84:MET:HG2	6:H:87:VAL:HG12	2.00	0.44
3:A:329:ILE:C	3:A:330:GLN:NE2	2.76	0.44
3:A:486:LEU:HA	3:A:528:LYS:HZ2	1.82	0.44
4:B:74:LEU:HD11	4:B:408:ALA:O	2.17	0.44
5:L:147:LYS:HB3	5:L:195:GLU:HB2	1.99	0.44
1:T:706:DT:H72	3:A:151:GLN:CG	2.48	0.44
3:A:255:ASN:HD22	3:A:289:LEU:HG	1.82	0.44
3:A:338:THR:CG2	3:A:339:TYR:N	2.81	0.44
4:B:156:SER:HB2	4:B:157:PRO:CD	2.48	0.44
4:B:312:GLU:CB	4:B:313:PRO:HD2	2.39	0.44
5:L:39:LYS:H	5:L:39:LYS:HG2	1.45	0.44
3:A:23:GLN:NE2	3:A:59:PRO:HA	2.33	0.43
3:A:184:MET:HB3	3:A:185:ASP:H	1.50	0.43
3:A:532:TYR:C	3:A:533:LEU:HD12	2.43	0.43
1:T:706:DT:O2	1:T:707:DG:C8	2.71	0.43
1:T:709:DC:H2'	1:T:710:DG:C8	2.53	0.43
3:A:31:ILE:C	3:A:33:ALA:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:331:LYS:HB3	3:A:421:PRO:HG2	1.99	0.43
4:B:58:THR:CG2	4:B:59:PRO:HD2	2.48	0.43
4:B:336:GLN:C	4:B:337:TRP:CD1	2.96	0.43
3:A:365:VAL:HG23	3:A:366:LYS:H	1.83	0.43
3:A:536:VAL:HG11	3:A:542:ILE:HG21	2.01	0.43
4:B:178:ILE:CG2	4:B:179:VAL:N	2.81	0.43
4:B:195:ILE:CG2	4:B:196:GLY:N	2.80	0.43
6:H:50:LEU:HD23	6:H:50:LEU:HA	1.85	0.43
4:B:12:LEU:HD11	4:B:127:TYR:OH	2.18	0.43
4:B:34:LEU:HA	4:B:34:LEU:HD12	1.69	0.43
4:B:153:TRP:CH2	4:B:155:GLY:HA3	2.53	0.43
4:B:254:VAL:O	4:B:257:ILE:N	2.47	0.43
5:L:33:LEU:CD2	5:L:34:ASN:N	2.81	0.43
3:A:366:LYS:O	3:A:367:GLN:C	2.61	0.43
3:A:443:ASP:CG	3:A:444:GLY:N	2.76	0.43
6:H:128:PRO:HA	6:H:209:HIS:CD2	2.49	0.43
3:A:263:LYS:O	3:A:266:TRP:HB3	2.19	0.43
3:A:293:ILE:CD1	3:A:294:PRO:HD2	2.43	0.43
3:A:543:GLY:O	3:A:545:ASN:N	2.50	0.43
4:B:330:GLN:HG2	4:B:338:THR:OG1	2.19	0.43
4:B:410:TRP:C	4:B:410:TRP:CE3	2.96	0.43
6:H:142:THR:HG22	6:H:144:SER:N	2.33	0.43
2:P:822[A]:TFO:N1	3:A:219:LYS:HD3	2.34	0.43
3:A:96:HIS:ND1	3:A:97:PRO:HD2	2.34	0.43
3:A:493:VAL:HG22	3:A:494:ASN:O	2.19	0.43
3:A:498:ASP:HB2	3:A:538:ALA:CB	2.41	0.43
4:B:116:PHE:HA	4:B:148:VAL:CG2	2.48	0.43
4:B:234:LEU:HD21	4:B:377:THR:HG21	2.01	0.43
5:L:182:THR:HG22	5:L:183:LYS:N	2.33	0.43
1:T:705:DA:C2	3:A:151:GLN:HG2	2.54	0.43
2:P:805:DG:H1'	2:P:806:DT:H5''	2.00	0.43
3:A:224:GLU:O	3:A:225:PRO:C	2.59	0.43
3:A:516:GLU:O	3:A:517:LEU:C	2.62	0.43
4:B:262:GLY:O	4:B:263:LYS:C	2.62	0.43
4:B:335:GLY:O	4:B:337:TRP:CD1	2.71	0.43
6:H:205:CYS:O	6:H:217:ASP:HA	2.18	0.43
3:A:456:GLY:O	3:A:548:VAL:CG1	2.67	0.43
4:B:63:ILE:HG13	4:B:63:ILE:O	2.18	0.43
3:A:106:VAL:CB	3:A:227:PHE:HE1	2.27	0.43
3:A:118:VAL:HG13	3:A:119:PRO:HD2	2.01	0.43
4:B:24:TRP:CZ3	4:B:59:PRO:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:76:ASP:O	4:B:78:ARG:N	2.49	0.43
4:B:100:LEU:HD21	4:B:106:VAL:HG21	2.01	0.43
4:B:252:TRP:CB	4:B:257:ILE:HD11	2.49	0.43
4:B:281:LYS:O	4:B:283:LEU:N	2.52	0.43
5:L:206:VAL:HG12	5:L:207:LYS:N	2.34	0.43
6:H:42:PRO:HA	6:H:93:ALA:HB2	2.01	0.43
6:H:199:PRO:O	6:H:200:SER:C	2.62	0.43
4:B:325:LEU:HD12	4:B:343:GLN:HG2	2.00	0.42
3:A:118:VAL:HA	3:A:119:PRO:HD3	1.79	0.42
3:A:139:THR:OG1	3:A:140:PRO:HD2	2.18	0.42
3:A:329:ILE:O	3:A:330:GLN:NE2	2.52	0.42
4:B:3:SER:HA	4:B:4:PRO:HD3	1.94	0.42
5:L:14:SER:O	5:L:15:LEU:C	2.62	0.42
6:H:42:PRO:HA	6:H:93:ALA:CB	2.48	0.42
4:B:50:ILE:HD13	4:B:145:GLN:HB3	2.01	0.42
4:B:342:TYR:HB3	4:B:348:ASN:HA	2.01	0.42
6:H:209:HIS:O	6:H:210:PRO:C	2.61	0.42
3:A:439:THR:O	3:A:441:TYR:HD1	2.02	0.42
3:A:542:ILE:CG2	3:A:543:GLY:N	2.82	0.42
4:B:223:LYS:CE	6:H:58:ASP:HB3	2.50	0.42
5:L:11:LEU:O	5:L:11:LEU:HG	2.12	0.42
5:L:81:GLU:O	5:L:82:ASP:C	2.63	0.42
6:H:39:ILE:HG21	6:H:47:LEU:HD22	2.00	0.42
6:H:47:LEU:HA	6:H:47:LEU:HD23	1.81	0.42
6:H:77:ASN:HB3	6:H:79:GLN:HG3	2.00	0.42
3:A:120:LEU:O	3:A:121:ASP:C	2.61	0.42
3:A:326:ILE:O	3:A:341:ILE:HA	2.19	0.42
3:A:329:ILE:HG13	3:A:391:LEU:HD22	2.02	0.42
3:A:516:GLU:O	3:A:520:GLN:N	2.47	0.42
4:B:60:VAL:HG11	4:B:75:VAL:HG22	2.00	0.42
4:B:178:ILE:HG22	4:B:179:VAL:N	2.33	0.42
4:B:242:GLN:NE2	4:B:242:GLN:CA	2.81	0.42
5:L:96:TRP:O	5:L:97:THR:HG23	2.20	0.42
6:H:69:LEU:O	6:H:70:THR:OG1	2.36	0.42
6:H:195:SER:C	6:H:197:THR:N	2.76	0.42
3:A:80:LEU:O	3:A:83:ARG:N	2.42	0.42
3:A:194:GLU:O	3:A:196:GLY:N	2.52	0.42
3:A:280:SER:C	3:A:282:LEU:N	2.78	0.42
3:A:303:LEU:O	3:A:307:ARG:HG3	2.20	0.42
3:A:466:VAL:CG2	3:A:551:LEU:HG	2.48	0.42
4:B:37:ILE:CD1	4:B:73:LYS:HB2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:146:TYR:CD2	4:B:150:PRO:CB	2.97	0.42
4:B:171:PHE:CZ	4:B:205:LEU:HB2	2.55	0.42
4:B:225:PRO:HB3	5:L:32:TYR:CZ	2.54	0.42
3:A:278:GLN:HB2	3:A:302:GLU:CB	2.49	0.42
3:A:296:THR:HG22	3:A:298:GLU:H	1.85	0.42
3:A:495:ILE:CG2	3:A:496:VAL:N	2.82	0.42
4:B:99:GLY:O	4:B:100:LEU:C	2.61	0.42
4:B:108:VAL:HG12	4:B:188:TYR:CD1	2.55	0.42
4:B:326:ILE:O	4:B:341:ILE:HA	2.20	0.42
5:L:89:GLN:HE21	5:L:89:GLN:HB3	1.52	0.42
5:L:142:LYS:O	5:L:144:ILE:N	2.53	0.42
6:H:12:VAL:HG12	6:H:13:GLN:O	2.19	0.42
3:A:125:ARG:O	3:A:126:LYS:C	2.62	0.42
4:B:135:ILE:HD12	4:B:135:ILE:C	2.44	0.42
3:A:222:GLN:C	3:A:224:GLU:N	2.75	0.42
3:A:317:VAL:CG1	3:A:349:LEU:HD23	2.49	0.42
3:A:390:LYS:C	3:A:391:LEU:HD23	2.45	0.42
3:A:417:VAL:O	3:A:417:VAL:HG13	2.20	0.42
3:A:464:GLN:O	3:A:465:LYS:HB2	2.20	0.42
4:B:55:PRO:HG2	4:B:56:TYR:CD1	2.55	0.42
4:B:249:LYS:HE3	4:B:256:ASP:OD2	2.20	0.42
6:H:12:VAL:HG12	6:H:13:GLN:N	2.34	0.42
6:H:88:GLU:HG2	6:H:91:ASP:OD2	2.20	0.42
3:A:115:TYR:C	3:A:117:SER:N	2.77	0.42
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.54	0.42
3:A:279:LEU:HA	3:A:282:LEU:HG	2.01	0.42
4:B:98:ALA:O	4:B:101:LYS:HE3	2.20	0.42
4:B:171:PHE:CE1	4:B:205:LEU:CA	3.01	0.42
4:B:195:ILE:HG23	4:B:196:GLY:N	2.34	0.42
4:B:353:LYS:HB2	4:B:353:LYS:NZ	2.35	0.42
5:L:109:ALA:O	5:L:110:ASP:C	2.63	0.42
6:H:56:ASP:OD2	6:H:58:ASP:HB2	2.19	0.42
3:A:222:GLN:O	3:A:223:LYS:C	2.62	0.41
3:A:339:TYR:CD2	3:A:375:ILE:HD11	2.54	0.41
3:A:457:TYR:HE1	3:A:484:LEU:HB3	1.86	0.41
3:A:458:VAL:CG2	3:A:548:VAL:HG13	2.45	0.41
3:A:516:GLU:O	3:A:519:ASN:N	2.53	0.41
4:B:97:PRO:CD	4:B:181:TYR:CD1	3.03	0.41
4:B:221:HIS:HB3	4:B:229:TRP:CD2	2.55	0.41
4:B:244:ILE:HD13	4:B:244:ILE:N	2.12	0.41
5:L:115:VAL:CG1	5:L:116:SER:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:148:TRP:CE3	5:L:179:LEU:HD13	2.55	0.41
1:T:706:DT:H2'	1:T:707:DG:C8	2.55	0.41
3:A:49:LYS:HE3	3:A:142:ILE:CG2	2.50	0.41
3:A:138:GLU:CG	3:A:139:THR:N	2.66	0.41
3:A:160:PHE:CD2	3:A:160:PHE:O	2.73	0.41
3:A:412:PRO:O	3:A:413:GLU:C	2.62	0.41
4:B:266:TRP:CZ2	4:B:422:LEU:HD13	2.55	0.41
5:L:140:TYR:CE2	5:L:141:PRO:HG3	2.54	0.41
5:L:185:GLU:HA	5:L:188:ARG:HB2	2.01	0.41
6:H:88:GLU:O	6:H:89:THR:C	2.63	0.41
6:H:88:GLU:O	6:H:121:VAL:HG21	2.20	0.41
3:A:132:ILE:HG22	3:A:142:ILE:O	2.21	0.41
3:A:260:LEU:O	3:A:264:LEU:HG	2.20	0.41
3:A:331:LYS:HD3	3:A:332:GLN:H	1.84	0.41
3:A:513:SER:OG	3:A:514:GLU:N	2.52	0.41
4:B:30:LYS:O	4:B:34:LEU:HB2	2.20	0.41
4:B:58:THR:HG22	4:B:59:PRO:N	2.36	0.41
6:H:92:THR:HG23	6:H:120:THR:CB	2.51	0.41
2:P:806:DT:H6	2:P:806:DT:H5'	1.85	0.41
3:A:306:ASN:O	3:A:307:ARG:C	2.62	0.41
3:A:481:ALA:C	3:A:483:TYR:N	2.77	0.41
4:B:38:CYS:O	4:B:41:MET:HB2	2.21	0.41
4:B:79:GLU:O	4:B:83:ARG:HG2	2.20	0.41
4:B:123:ASP:O	4:B:125:ARG:N	2.53	0.41
5:L:82:ASP:O	5:L:84:ALA:N	2.54	0.41
3:A:121:ASP:C	3:A:121:ASP:OD1	2.64	0.41
3:A:171:PHE:CZ	3:A:205:LEU:HB2	2.55	0.41
3:A:465:LYS:CE	3:A:488:ASP:OD2	2.68	0.41
4:B:18:GLY:H	4:B:56:TYR:HE2	1.68	0.41
5:L:98:PHE:CZ	6:H:39:ILE:HD12	2.55	0.41
3:A:363:ASN:CB	3:A:511:ASP:HB3	2.50	0.41
3:A:445:ALA:N	3:A:477:THR:OG1	2.53	0.41
4:B:337:TRP:CD1	4:B:337:TRP:N	2.88	0.41
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.77	0.41
6:H:24:PHE:CD1	6:H:24:PHE:C	2.99	0.41
3:A:17:ASP:O	3:A:83:ARG:NH1	2.53	0.41
3:A:260:LEU:O	3:A:261:VAL:C	2.63	0.41
3:A:279:LEU:CD2	3:A:279:LEU:N	2.81	0.41
3:A:481:ALA:O	3:A:483:TYR:N	2.53	0.41
6:H:56:ASP:O	6:H:57:ASP:HB2	2.21	0.41
6:H:163:THR:C	6:H:206:ASN:HD22	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:61:PHE:CD2	3:A:61:PHE:N	2.80	0.41
3:A:459:THR:HG23	3:A:462:GLY:H	1.86	0.41
4:B:373:GLN:HE22	4:B:407:GLN:H	1.69	0.41
4:B:421:PRO:O	4:B:422:LEU:C	2.63	0.41
3:A:183:TYR:CE2	3:A:230:MET:HE1	2.56	0.41
3:A:365:VAL:O	3:A:366:LYS:C	2.63	0.41
3:A:494:ASN:N	3:A:494:ASN:HD22	2.18	0.41
3:A:499:SER:OG	3:A:502:ALA:HB3	2.19	0.41
3:A:536:VAL:HG11	3:A:542:ILE:CG2	2.51	0.41
4:B:2:ILE:CD1	4:B:3:SER:N	2.77	0.41
4:B:74:LEU:HD21	4:B:409:THR:O	2.21	0.41
4:B:101:LYS:O	4:B:236:PRO:CB	2.69	0.41
4:B:153:TRP:O	4:B:154:LYS:C	2.63	0.41
4:B:221:HIS:HB3	4:B:229:TRP:CE2	2.55	0.41
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.56	0.41
5:L:98:PHE:CZ	6:H:110:MET:HE1	2.56	0.41
6:H:155:TYR:CD2	6:H:185:TYR:O	2.73	0.41
1:T:713:DC:H2'	1:T:714:DG:C8	2.56	0.40
3:A:235:HIS:CE1	3:A:240:THR:HG22	2.56	0.40
3:A:389:PHE:HB3	3:A:391:LEU:HD21	2.03	0.40
3:A:502:ALA:O	3:A:506:ILE:HG12	2.21	0.40
4:B:149:LEU:HD11	4:B:159:ILE:CG2	2.51	0.40
4:B:202:ILE:C	4:B:204:GLU:N	2.79	0.40
4:B:266:TRP:CH2	4:B:422:LEU:HD13	2.55	0.40
5:L:106:ILE:HG12	5:L:166:GLN:CD	2.44	0.40
3:A:31:ILE:O	3:A:33:ALA:N	2.54	0.40
3:A:84:THR:O	3:A:85:GLN:C	2.64	0.40
3:A:439:THR:HB	4:B:289:LEU:HG	2.03	0.40
4:B:104:LYS:HD2	4:B:192:ASP:O	2.20	0.40
5:L:58:VAL:HG13	5:L:59:PRO:HD2	2.04	0.40
5:L:83:ILE:CG2	5:L:104:LEU:O	2.69	0.40
6:H:195:SER:O	6:H:197:THR:N	2.54	0.40
3:A:31:ILE:O	3:A:35:VAL:HG23	2.22	0.40
3:A:115:TYR:O	3:A:117:SER:N	2.54	0.40
3:A:143:ARG:HG3	3:A:143:ARG:NH1	2.35	0.40
3:A:194:GLU:C	3:A:196:GLY:N	2.78	0.40
3:A:244:ILE:CG1	3:A:263:LYS:HD3	2.49	0.40
3:A:365:VAL:HG21	3:A:401:TRP:CE2	2.56	0.40
3:A:463:ARG:C	3:A:464:GLN:HE21	2.29	0.40
4:B:118:VAL:H	4:B:148:VAL:HG23	1.86	0.40
4:B:273:GLY:C	4:B:274:ILE:HD13	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:325:LEU:HB3	4:B:387:PRO:CA	2.51	0.40
4:B:329:ILE:HG22	4:B:392:PRO:HG3	2.04	0.40
5:L:51:THR:OG1	5:L:71:TYR:HD2	2.04	0.40
6:H:7:SER:HB2	6:H:21:THR:HB	2.02	0.40
6:H:71:VAL:HG12	6:H:72:SER:N	2.37	0.40
6:H:94:ILE:HA	6:H:117:THR:O	2.22	0.40
3:A:27:THR:O	3:A:31:ILE:HG13	2.21	0.40
3:A:365:VAL:HG23	3:A:366:LYS:N	2.36	0.40
3:A:546:GLU:O	3:A:547:GLN:C	2.64	0.40
4:B:74:LEU:HD23	4:B:74:LEU:HA	1.85	0.40
4:B:98:ALA:O	4:B:101:LYS:HG2	2.22	0.40
5:L:190:ASN:HA	5:L:211:ARG:HG2	2.04	0.40
3:A:168:LEU:HA	3:A:168:LEU:HD23	1.87	0.40
3:A:194:GLU:C	3:A:196:GLY:H	2.28	0.40
3:A:262:GLY:O	3:A:265:ASN:HB2	2.22	0.40
3:A:320:ASP:HA	3:A:321:PRO:HD3	1.93	0.40
3:A:342:TYR:HD1	3:A:342:TYR:H	1.69	0.40
3:A:398:TRP:O	3:A:401:TRP:N	2.53	0.40
4:B:125:ARG:HD3	4:B:147:ASN:HA	2.02	0.40
4:B:237:ASP:O	4:B:239:TRP:N	2.52	0.40
6:H:22:CYS:HB3	6:H:80:ALA:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2:ILE:O	4:B:2:ILE:O[6_565]	1.67	0.53

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	
3	A	556/558 (100%)	431 (78%)	92 (16%)	33 (6%)	1	8
4	B	427/437 (98%)	324 (76%)	75 (18%)	28 (7%)	1	6
5	L	209/211 (99%)	165 (79%)	34 (16%)	10 (5%)	2	11
6	H	223/225 (99%)	185 (83%)	23 (10%)	15 (7%)	1	6
All	All	1415/1431 (99%)	1105 (78%)	224 (16%)	86 (6%)	1	7

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	67	ASP
3	A	138	GLU
3	A	273	GLY
3	A	466	VAL
3	A	474	ASN
3	A	528	LYS
3	A	543	GLY
4	B	2	ILE
4	B	124	PHE
4	B	225	PRO
4	B	247	PRO
4	B	286	THR
4	B	315	HIS
5	L	51	THR
5	L	76	SER
5	L	78	LEU
5	L	110	ASP
5	L	143	ASP
6	H	140	ALA
6	H	202	THR
3	A	66	LYS
3	A	116	PHE
3	A	284	ARG
3	A	324	ASP
3	A	458	VAL
3	A	459	THR
3	A	465	LYS
3	A	485	ALA
3	A	547	GLN
4	B	77	PHE
4	B	116	PHE
4	B	154	LYS
4	B	355	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	17	ASP
6	H	10	GLY
6	H	32	SER
3	A	376	THR
3	A	508	ALA
3	A	530	LYS
4	B	111	VAL
4	B	282	LEU
6	H	59	ASN
6	H	126	THR
6	H	139	ALA
6	H	143	ASN
6	H	166	SER
3	A	85	GLN
3	A	114	ALA
3	A	281	LYS
4	B	5	ILE
4	B	170	PRO
4	B	300	GLU
4	B	422	LEU
4	B	424	LYS
6	H	86	THR
6	H	170	SER
6	H	200	SER
3	A	123	ASP
3	A	140	PRO
3	A	243	PRO
3	A	249	LYS
3	A	278	GLN
3	A	286	THR
3	A	463	ARG
4	B	44	GLU
4	B	87	PHE
4	B	95	PRO
4	B	226	PRO
4	B	238	LYS
4	B	270	ILE
5	L	82	ASP
3	A	544	GLY
4	B	140	PRO
4	B	232	TYR
4	B	421	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	83	ILE
5	L	152	GLY
3	A	195	ILE
5	L	68	GLY
6	H	34	ILE
6	H	210	PRO
4	B	156	SER
3	A	321	PRO
4	B	314	VAL
3	A	505	ILE
6	H	159	PRO

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	
3	A	485/498 (97%)	437 (90%)	48 (10%)	7	29
4	B	388/397 (98%)	344 (89%)	44 (11%)	5	23
5	L	190/190 (100%)	177 (93%)	13 (7%)	14	42
6	H	196/196 (100%)	173 (88%)	23 (12%)	5	22
All	All	1259/1281 (98%)	1131 (90%)	128 (10%)	7	28

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	34	LEU
3	A	37	ILE
3	A	38	CYS
3	A	49	LYS
3	A	55	PRO
3	A	61	PHE
3	A	80	LEU
3	A	85	GLN
3	A	86	ASP
3	A	94	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	122	GLU
3	A	132	ILE
3	A	175	ASN
3	A	179	VAL
3	A	215	THR
3	A	220	LYS
3	A	246	LEU
3	A	325	LEU
3	A	331	LYS
3	A	342	TYR
3	A	365	VAL
3	A	373	GLN
3	A	376	THR
3	A	385	LYS
3	A	387	PRO
3	A	397	THR
3	A	401	TRP
3	A	409	THR
3	A	410	TRP
3	A	415	GLU
3	A	439	THR
3	A	454	LYS
3	A	464	GLN
3	A	469	LEU
3	A	477	THR
3	A	478	GLU
3	A	497	THR
3	A	500	GLN
3	A	503	LEU
3	A	511	ASP
3	A	525	LEU
3	A	532	TYR
3	A	533	LEU
3	A	545	ASN
3	A	547	GLN
3	A	548	VAL
3	A	550	LYS
3	A	552	VAL
4	B	12	LEU
4	B	37	ILE
4	B	42	GLU
4	B	47	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	55	PRO
4	B	95	PRO
4	B	106	VAL
4	B	109	LEU
4	B	148	VAL
4	B	175	ASN
4	B	193	LEU
4	B	200	THR
4	B	212	TRP
4	B	215	THR
4	B	216	THR
4	B	218	ASP
4	B	225	PRO
4	B	233	GLU
4	B	234	LEU
4	B	244	ILE
4	B	250	ASP
4	B	271	TYR
4	B	276	VAL
4	B	286	THR
4	B	295	LEU
4	B	300	GLU
4	B	301	LEU
4	B	305	GLU
4	B	315	HIS
4	B	324	ASP
4	B	330	GLN
4	B	332	GLN
4	B	340	GLN
4	B	351	THR
4	B	353	LYS
4	B	364	ASP
4	B	386	THR
4	B	387	PRO
4	B	396	GLU
4	B	401	TRP
4	B	407	GLN
4	B	410	TRP
4	B	419	THR
4	B	423	VAL
5	L	7	THR
5	L	8	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	11	LEU
5	L	33	LEU
5	L	39	LYS
5	L	49	TYR
5	L	69	THR
5	L	77	ASN
5	L	89	GLN
5	L	97	THR
5	L	108	ARG
5	L	110	ASP
5	L	197	THR
6	H	3	THR
6	H	4	LEU
6	H	23	THR
6	H	29	LEU
6	H	43	SER
6	H	59	ASN
6	H	72	SER
6	H	82	LEU
6	H	88	GLU
6	H	107	ASP
6	H	123	SER
6	H	129	PRO
6	H	152	VAL
6	H	157	PRO
6	H	159	PRO
6	H	160	VAL
6	H	163	THR
6	H	186	THR
6	H	187	LEU
6	H	192	THR
6	H	200	SER
6	H	215	LYS
6	H	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	GLN
3	A	85	GLN
3	A	147	ASN
3	A	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	207	GLN
3	A	222	GLN
3	A	235	HIS
3	A	255	ASN
3	A	265	ASN
3	A	269	GLN
3	A	306	ASN
3	A	330	GLN
3	A	340	GLN
3	A	343	GLN
3	A	367	GLN
3	A	447	ASN
3	A	464	GLN
3	A	494	ASN
3	A	500	GLN
3	A	539	HIS
4	B	57	ASN
4	B	151	GLN
4	B	161	GLN
4	B	175	ASN
4	B	222	GLN
4	B	235	HIS
4	B	242	GLN
4	B	255	ASN
4	B	258	GLN
4	B	315	HIS
4	B	330	GLN
4	B	363	ASN
4	B	367	GLN
4	B	373	GLN
4	B	418	ASN
5	L	27	GLN
5	L	77	ASN
5	L	89	GLN
5	L	90	GLN
5	L	124	GLN
5	L	138	ASN
5	L	190	ASN
5	L	210	ASN
6	H	59	ASN
6	H	62	ASN
6	H	174	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	206	ASN
6	H	209	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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
2	TFO	P	822[A]	2	15,19,20	3.08	9 (60%)	20,26,29	6.21	10 (50%)
2	TFO	P	822[B]	2	15,19,20	0.51	0	20,26,29	1.77	3 (15%)
2	MRG	P	817	2,1	21,24,29	0.42	0	30,35,42	0.61	1 (3%)

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
2	TFO	P	822[A]	2	-	4/7/9/10	0/2/2/2
2	TFO	P	822[B]	2	-	2/7/9/10	0/2/2/2
2	MRG	P	817	2,1	-	0/7/21/27	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	822[A]	TFO	C8'-C7'	5.77	1.73	1.51
2	P	822[A]	TFO	C6'-N9	-5.15	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	822[A]	TFO	O9'-C7'	-4.65	1.36	1.44
2	P	822[A]	TFO	C4-N9	-4.32	1.32	1.37
2	P	822[A]	TFO	C8-N9	3.62	1.42	1.36
2	P	822[A]	TFO	C2-N3	-3.19	1.28	1.33
2	P	822[A]	TFO	C5-C4	-2.70	1.34	1.39
2	P	822[A]	TFO	C8-N7	2.35	1.36	1.31
2	P	822[A]	TFO	C4-N3	-2.17	1.30	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	822[A]	TFO	C7'-C6'-N9	22.06	147.53	112.68
2	P	822[A]	TFO	C6'-N9-C4	-9.87	114.95	126.41
2	P	822[A]	TFO	C6'-N9-C8	7.24	138.20	126.63
2	P	822[A]	TFO	N3-C4-N9	-7.05	118.15	126.87
2	P	822[B]	TFO	C7'-C6'-N9	5.44	121.28	112.68
2	P	822[A]	TFO	N9-C8-N7	-5.18	109.37	114.16
2	P	822[B]	TFO	C6'-N9-C4	4.77	131.93	126.41
2	P	822[A]	TFO	C5-C4-N3	4.48	132.88	126.72
2	P	822[A]	TFO	C6-C5-C4	-3.61	112.25	117.18
2	P	822[B]	TFO	C6'-N9-C8	-2.90	121.99	126.63
2	P	817	MRG	O3'-C3'-C2'	-2.84	101.00	110.88
2	P	822[A]	TFO	C5-C4-N9	2.77	108.82	105.98
2	P	822[A]	TFO	C6-C5-N7	2.34	136.60	132.09
2	P	822[A]	TFO	N1-C2-N3	-2.07	125.45	128.58

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	822[A]	TFO	N9-C6'-C7'-O9'
2	P	822[A]	TFO	N9-C6'-C7'-C8'
2	P	822[A]	TFO	C7'-C6'-N9-C4
2	P	822[B]	TFO	C7'-C6'-N9-C4
2	P	822[A]	TFO	C7'-C6'-N9-C8
2	P	822[B]	TFO	C7'-C6'-N9-C8

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	822[A]	TFO	2	0
2	P	822[B]	TFO	5	0
2	P	817	MRG	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	T	23/27 (85%)	0.59	2 (8%)	16 9	53, 99, 132, 135	0
2	P	18/21 (85%)	0.33	1 (5%)	30 16	33, 87, 109, 121	1 (5%)
3	A	556/558 (99%)	-0.00	12 (2%)	62 41	16, 69, 117, 131	1 (0%)
4	B	429/437 (98%)	-0.31	5 (1%)	76 58	15, 48, 112, 128	1 (0%)
5	L	211/211 (100%)	-0.25	0	100 100	26, 60, 105, 116	0
6	H	225/225 (100%)	-0.41	3 (1%)	75 56	16, 48, 92, 129	0
All	All	1462/1479 (98%)	-0.18	23 (1%)	70 49	15, 58, 113, 135	3 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	556	ILE	4.9
3	A	1	PRO	4.3
4	B	429	LEU	3.5
3	A	222	GLN	3.5
1	T	705	DA	3.2
4	B	428	GLN	3.0
3	A	356	ARG	2.8
4	B	88	TRP	2.7
3	A	544	GLY	2.7
6	H	137	GLY	2.6
3	A	461	LYS	2.6
3	A	425	LEU	2.5
3	A	448	ARG	2.4
3	A	240	THR	2.4
3	A	223	LYS	2.4
2	P	821[A]	DC	2.4
4	B	334	GLN	2.3
1	T	704	DC	2.3
3	A	434	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	315	HIS	2.2
6	H	138	SER	2.2
6	H	139	ALA	2.1
3	A	426	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TFO	P	822[A]	18/19	0.72	0.44	85,98,98,98	18
2	TFO	P	822[B]	18/19	0.72	0.44	86,98,98,98	18
2	MRG	P	817	22/27	0.87	0.12	97,109,112,115	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
7	MG	A	559	1/1	0.99	0.14	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.