



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:52 AM UTC

PDB ID : 1IJS / pdb_00001ijs
Title : CPV (STRAIN D) mutant A300D, complex (VIRAL COAT/DNA), VP2, PH=7.5, T=4 DEGREES C
Authors : Llamas-Saiz, A.L.; Agbandje-McKenna, M.; Parker, J.S.L.; Wahid, A.T.M.; Parrish, C.R.; Rossmann, M.G.
Deposited on : 1996-09-12
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

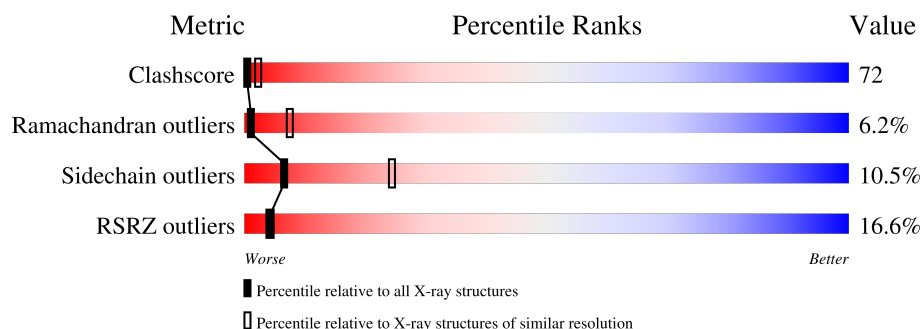
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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))
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	N	9	33% 33% 67%
2	A	2	100%
3	P	584	15% 28% 48% 15% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4571 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 DNA (5'-D(*CP*CP*AP*CP*CP*CP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	9	Total	C	N	O	P	0	0	0
			178	84	33	52	9			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	P	0	0	0
			40	19	8	11	2			

- Molecule 3 is a protein called PROTEIN (PARVOVIRUS COAT PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	548	Total	C	N	O	S	0	0	0
			4353	2765	742	830	16			

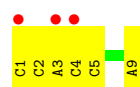
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	300	ASP	ALA	engineered mutation	UNP P30129
P	386	GLN	LYS	conflict	UNP P30129

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.

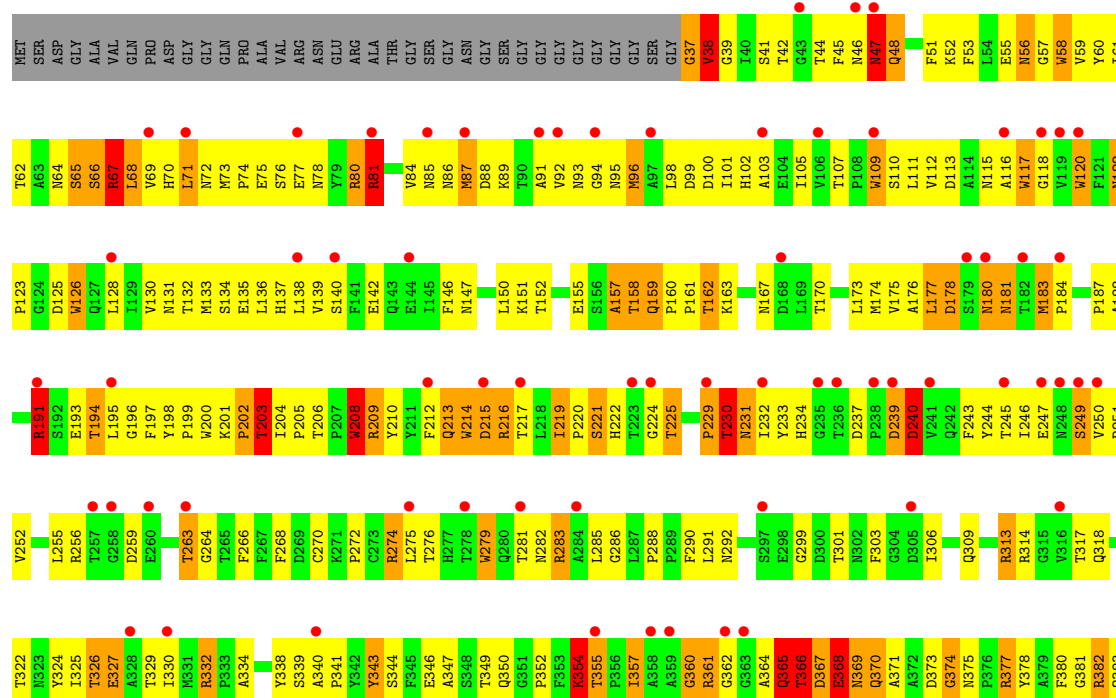
- Molecule 1: DNA (5'-D(*CP*CP*AP*CP*CP*CP*CP*AP*A)-3')

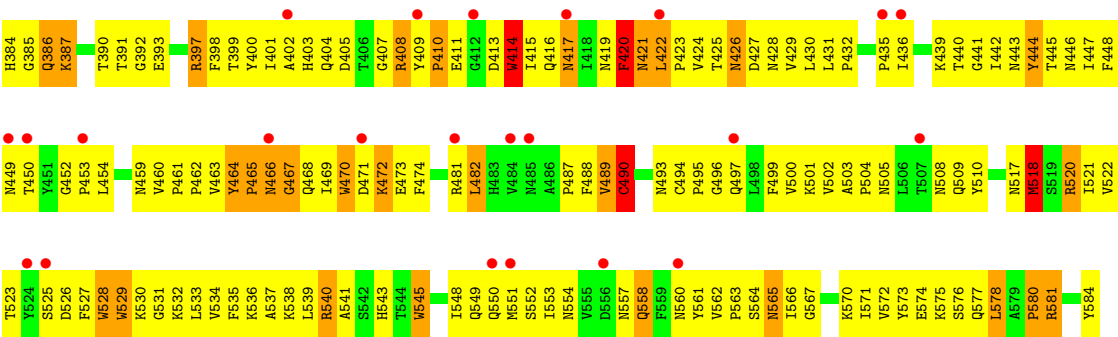


- Molecule 2: DNA (5'-D(*AP*C)-3')



- Molecule 3: PROTEIN (PARVOVIRUS COAT PROTEIN)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	267.60Å 268.50Å 274.30Å 61.90° 62.60° 60.20°	Depositor
Resolution (Å)	(Not available) – 3.25 200.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.25) 32.2 (200.00-3.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.97 (at 3.25Å)	Xtriage
Refinement program	NONE	Depositor
R, R_{free}	(Not available) , (Not available) 0.529 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for -h+k,-h,-h+l 0.014 for -k,h-k,-k+l 0.028 for h,h-k,h-l 0.035 for -h+k,k,k-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.06	EDS
Total number of atoms	4571	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	N	0.81	1/198 (0.5%)	0.94	0/299
2	A	0.54	0/44	0.87	0/65
3	P	1.39	42/4483 (0.9%)	1.35	38/6133 (0.6%)
All	All	1.36	43/4725 (0.9%)	1.33	38/6497 (0.6%)

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
3	P	0	1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	490	CYS	CA-C	19.62	1.77	1.52
3	P	490	CYS	N-CA	-16.10	1.26	1.46
3	P	81	ARG	CD-NE	15.01	1.67	1.46
3	P	239	ASP	C-N	-13.03	1.15	1.33
3	P	252	VAL	N-CA	-10.21	1.34	1.46
3	P	496	GLY	C-N	-9.63	1.20	1.33
3	P	203	THR	N-CA	8.78	1.57	1.45
3	P	47	ASN	C-N	-8.15	1.22	1.33
3	P	497	GLN	N-CA	-7.41	1.36	1.46
3	P	251	PRO	C-N	-7.32	1.24	1.33
3	P	38	VAL	N-CA	7.14	1.55	1.46
3	P	203	THR	C-N	6.95	1.41	1.33
3	P	326	THR	CA-C	6.80	1.61	1.52
3	P	240	ASP	N-CA	-6.72	1.37	1.46
3	P	327	GLU	N-CA	6.18	1.54	1.46
3	P	80	ARG	C-N	-6.15	1.25	1.33
3	P	208	TRP	NE1-CE2	-6.05	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	178	ASP	CA-C	-5.82	1.47	1.53
3	P	214	TRP	NE1-CE2	-5.77	1.31	1.37
3	P	354	LYS	N-CA	5.77	1.53	1.45
3	P	202	PRO	CA-C	5.73	1.59	1.52
3	P	162	THR	N-CA	5.69	1.53	1.45
3	P	202	PRO	C-N	5.55	1.43	1.33
3	P	251	PRO	C-O	5.53	1.30	1.23
3	P	290	PHE	C-N	-5.53	1.25	1.33
3	P	414	TRP	NE1-CE2	-5.52	1.31	1.37
1	N	1	DC	OP3-P	5.50	1.59	1.48
3	P	117	TRP	NE1-CE2	-5.48	1.31	1.37
3	P	470	TRP	NE1-CE2	-5.44	1.31	1.37
3	P	529	TRP	NE1-CE2	-5.43	1.31	1.37
3	P	126	TRP	NE1-CE2	-5.40	1.31	1.37
3	P	279	TRP	NE1-CE2	-5.40	1.31	1.37
3	P	528	TRP	NE1-CE2	-5.39	1.31	1.37
3	P	210	TYR	N-CA	5.38	1.52	1.45
3	P	37	GLY	CA-C	5.37	1.61	1.52
3	P	545	TRP	NE1-CE2	-5.36	1.31	1.37
3	P	58	TRP	NE1-CE2	-5.34	1.31	1.37
3	P	109	TRP	NE1-CE2	-5.31	1.31	1.37
3	P	200	TRP	NE1-CE2	-5.30	1.31	1.37
3	P	263	THR	C-N	-5.30	1.25	1.33
3	P	251	PRO	CA-C	-5.14	1.45	1.52
3	P	120	TRP	NE1-CE2	-5.08	1.31	1.37
3	P	48	GLN	C-N	-5.07	1.25	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	490	CYS	N-CA-CB	13.87	130.77	109.83
3	P	81	ARG	CG-CD-NE	11.47	137.24	112.00
3	P	81	ARG	CA-CB-CG	8.43	130.96	114.10
3	P	47	ASN	CA-C-N	6.06	131.72	122.93
3	P	47	ASN	C-N-CA	6.06	131.72	122.93
3	P	490	CYS	CA-C-O	-6.00	114.59	121.19
3	P	343	TYR	CB-CA-C	5.84	119.57	111.63
3	P	194	THR	CB-CA-C	-5.77	108.76	117.07
3	P	81	ARG	NE-CZ-NH2	5.75	124.37	119.20
3	P	281	THR	CB-CA-C	-5.75	108.79	117.07
3	P	38	VAL	CB-CA-C	-5.75	101.87	111.29
3	P	314	ARG	NE-CZ-NH2	5.52	124.17	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	361	ARG	NE-CZ-NH2	5.48	124.13	119.20
3	P	368	GLU	O-C-N	5.46	129.85	122.59
3	P	216	ARG	NE-CZ-NH2	5.43	124.09	119.20
3	P	209	ARG	NE-CZ-NH2	5.42	124.08	119.20
3	P	274	ARG	NE-CZ-NH2	5.38	124.04	119.20
3	P	382	ARG	NE-CZ-NH2	5.37	124.04	119.20
3	P	67	ARG	NE-CZ-NH2	5.36	124.03	119.20
3	P	581	ARG	NE-CZ-NH2	5.36	124.02	119.20
3	P	191	ARG	NE-CZ-NH2	5.36	124.02	119.20
3	P	80	ARG	NE-CZ-NH2	5.34	124.00	119.20
3	P	332	ARG	NE-CZ-NH2	5.32	123.99	119.20
3	P	540	ARG	NE-CZ-NH2	5.31	123.98	119.20
3	P	313	ARG	NE-CZ-NH2	5.31	123.98	119.20
3	P	256	ARG	NE-CZ-NH2	5.31	123.98	119.20
3	P	481	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	P	520	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	P	283	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	P	408	ARG	NE-CZ-NH2	5.27	123.94	119.20
3	P	397	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	P	377	ARG	NE-CZ-NH2	5.19	123.87	119.20
3	P	194	THR	O-C-N	5.19	125.36	121.47
3	P	580	PRO	O-C-N	5.14	128.88	122.71
3	P	489	VAL	CA-C-N	5.14	128.01	120.71
3	P	489	VAL	C-N-CA	5.14	128.01	120.71
3	P	281	THR	CA-C-O	5.13	120.92	117.94
3	P	444	TYR	N-CA-C	-5.05	106.97	113.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	81	ARG	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	N	178	0	99	7	0
2	A	40	0	23	12	0
3	P	4353	0	4144	621	0
All	All	4571	0	4266	640	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 72.

All (640) 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:P:96:MET:CE	3:P:221:SER:H	1.02	1.57
3:P:490:CYS:C	3:P:490:CYS:CA	1.77	1.54
3:P:424:VAL:HG21	3:P:429:VAL:CG2	1.35	1.51
2:A:1:DA:C3'	2:A:2:DC:H5''	1.48	1.44
3:P:276:THR:CG2	3:P:581:ARG:HB2	1.48	1.44
2:A:1:DA:C2'	2:A:2:DC:H5''	1.44	1.44
3:P:424:VAL:CG2	3:P:429:VAL:CG2	2.00	1.40
3:P:70:HIS:CD2	3:P:526:ASP:OD2	1.74	1.38
3:P:150:LEU:CD2	3:P:525:SER:HB3	1.54	1.38
3:P:96:MET:CE	3:P:221:SER:N	1.83	1.37
3:P:159:GLN:HB2	3:P:160:PRO:CD	1.53	1.32
3:P:130:VAL:CG1	3:P:578:LEU:HD21	1.60	1.30
3:P:158:THR:O	3:P:160:PRO:HD2	1.25	1.28
3:P:113:ASP:O	3:P:195:LEU:CD1	1.84	1.26
3:P:150:LEU:HD23	3:P:525:SER:CB	1.63	1.26
3:P:70:HIS:HD2	3:P:526:ASP:OD2	0.95	1.25
3:P:113:ASP:O	3:P:195:LEU:HD12	1.33	1.25
3:P:75:GLU:CG	3:P:76:SER:H	1.43	1.24
3:P:96:MET:HE2	3:P:221:SER:N	1.43	1.24
3:P:111:LEU:HD23	3:P:112:VAL:N	1.52	1.24
3:P:505:ASN:OD1	3:P:521:ILE:HD12	1.38	1.23
3:P:160:PRO:CB	3:P:161:PRO:O	1.87	1.21
3:P:75:GLU:HG3	3:P:76:SER:N	1.53	1.19
3:P:424:VAL:CG2	3:P:429:VAL:HG23	1.63	1.16
3:P:263:THR:HG22	3:P:264:GLY:H	1.11	1.14
3:P:361:ARG:O	3:P:373:ASP:OD2	1.66	1.14
3:P:193:GLU:HB3	3:P:206:THR:HG21	1.21	1.12
3:P:109:TRP:NE1	3:P:247:GLU:OE2	1.82	1.12
3:P:160:PRO:HB2	3:P:161:PRO:O	0.95	1.11
3:P:424:VAL:HG22	3:P:429:VAL:HG23	1.26	1.11
2:A:1:DA:C2'	2:A:2:DC:C5'	2.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:365:GLN:OE1	3:P:365:GLN:HA	1.46	1.09
3:P:424:VAL:HG21	3:P:429:VAL:HG21	1.32	1.09
3:P:361:ARG:HG2	3:P:362:GLY:H	1.04	1.08
3:P:75:GLU:HG2	3:P:76:SER:H	1.08	1.08
3:P:134:SER:O	3:P:275:LEU:HB2	1.53	1.08
3:P:174:MET:HE3	3:P:503:ALA:HA	1.33	1.07
3:P:194:THR:HG22	3:P:195:LEU:H	1.12	1.07
3:P:361:ARG:CG	3:P:362:GLY:H	1.66	1.07
3:P:96:MET:HE3	3:P:221:SER:H	1.15	1.07
3:P:276:THR:CG2	3:P:581:ARG:CB	2.31	1.06
3:P:276:THR:HG21	3:P:581:ARG:CB	1.83	1.06
3:P:367:ASP:OD2	3:P:409:TYR:CE2	2.09	1.05
3:P:517:ASN:O	3:P:518:MET:O	1.74	1.05
2:A:1:DA:H2''	2:A:2:DC:O4'	1.55	1.04
3:P:130:VAL:HG12	3:P:578:LEU:HD21	1.32	1.04
3:P:381:GLY:HA2	3:P:386:GLN:NE2	1.70	1.04
3:P:193:GLU:HB3	3:P:206:THR:CG2	1.87	1.04
3:P:75:GLU:CG	3:P:76:SER:N	2.01	1.04
2:A:1:DA:C3'	2:A:2:DC:C5'	2.35	1.04
3:P:75:GLU:O	3:P:520:ARG:NH2	1.91	1.03
3:P:424:VAL:HG21	3:P:429:VAL:HG22	1.35	1.03
2:A:1:DA:H2''	2:A:2:DC:C4'	1.89	1.03
3:P:157:ALA:HA	3:P:161:PRO:HB3	1.35	1.02
3:P:52:LYS:HB3	3:P:60:TYR:HB3	1.38	1.01
3:P:159:GLN:CB	3:P:160:PRO:HD3	1.88	1.01
3:P:465:PRO:HG3	3:P:571:ILE:CG2	1.89	1.01
2:A:1:DA:H2''	2:A:2:DC:C5'	1.90	1.01
2:A:1:DA:H2''	2:A:2:DC:H5''	1.38	1.01
3:P:101:ILE:HG21	3:P:216:ARG:HD2	1.44	1.00
3:P:74:PRO:O	3:P:520:ARG:NH2	1.94	1.00
2:A:1:DA:H3'	2:A:2:DC:H5''	1.39	1.00
3:P:213:GLN:OE1	3:P:237:ASP:HB2	1.63	0.99
3:P:431:LEU:HB3	3:P:432:PRO:HD2	1.45	0.98
3:P:96:MET:HE2	3:P:220:PRO:C	1.88	0.98
3:P:96:MET:HE1	3:P:221:SER:H	1.30	0.97
3:P:118:GLY:HA3	3:P:197:PHE:CE2	1.99	0.96
3:P:96:MET:HE2	3:P:220:PRO:CA	1.96	0.96
3:P:367:ASP:OD2	3:P:409:TYR:HE2	1.41	0.95
3:P:96:MET:HE2	3:P:221:SER:H	1.00	0.95
3:P:53:PHE:CD1	3:P:59:VAL:HG22	2.02	0.95
3:P:429:VAL:HG12	3:P:431:LEU:CD1	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:370:GLN:HE21	3:P:399:THR:HG21	1.30	0.94
3:P:158:THR:O	3:P:160:PRO:CD	2.15	0.94
3:P:99:ASP:CG	3:P:216:ARG:NH1	2.26	0.94
3:P:381:GLY:HA2	3:P:386:GLN:HE21	1.26	0.93
3:P:38:VAL:HG22	3:P:38:VAL:O	1.64	0.93
3:P:465:PRO:HG3	3:P:571:ILE:HG21	1.48	0.93
3:P:365:GLN:OE1	3:P:365:GLN:CA	2.16	0.93
3:P:197:PHE:HE2	3:P:465:PRO:HB2	1.33	0.92
3:P:276:THR:HG21	3:P:581:ARG:HB2	0.93	0.92
3:P:466:ASN:O	3:P:467:GLY:O	1.88	0.92
3:P:443:ASN:HB2	3:P:446:ASN:OD1	1.68	0.92
3:P:99:ASP:OD2	3:P:216:ARG:NH1	2.02	0.91
3:P:159:GLN:HB2	3:P:160:PRO:HD3	0.92	0.91
3:P:193:GLU:CB	3:P:206:THR:HG21	2.01	0.90
3:P:322:THR:CG2	3:P:420:PHE:CD2	2.55	0.90
3:P:219:ILE:HG13	3:P:230:THR:HB	1.54	0.90
3:P:131:ASN:HD21	3:P:551:MET:HB3	1.37	0.89
3:P:73:MET:CE	3:P:520:ARG:HG3	2.02	0.89
3:P:77:GLU:HG2	3:P:520:ARG:NH1	1.88	0.89
3:P:361:ARG:CG	3:P:362:GLY:N	2.30	0.89
3:P:469:ILE:CG2	3:P:470:TRP:HE3	1.86	0.89
3:P:38:VAL:O	3:P:38:VAL:CG2	2.20	0.89
3:P:361:ARG:HG2	3:P:362:GLY:N	1.86	0.88
3:P:160:PRO:HB2	3:P:161:PRO:C	1.98	0.88
3:P:73:MET:HE1	3:P:520:ARG:HG3	1.54	0.88
3:P:274:ARG:HD3	3:P:581:ARG:HH12	1.39	0.88
3:P:194:THR:HG22	3:P:195:LEU:N	1.89	0.88
3:P:73:MET:HE3	3:P:520:ARG:NE	1.88	0.88
3:P:416:GLN:HB3	3:P:429:VAL:HG22	1.55	0.88
3:P:130:VAL:CG1	3:P:578:LEU:CD2	2.50	0.87
3:P:279:TRP:HE3	3:P:279:TRP:O	1.58	0.87
3:P:424:VAL:CG2	3:P:429:VAL:HG21	1.89	0.87
3:P:263:THR:CG2	3:P:264:GLY:H	1.88	0.86
3:P:157:ALA:HA	3:P:161:PRO:CB	2.05	0.86
1:N:3:DA:H5'	1:N:9:DA:H5''	1.58	0.86
3:P:469:ILE:CG2	3:P:470:TRP:CE3	2.59	0.86
3:P:505:ASN:OD1	3:P:521:ILE:CD1	2.23	0.85
3:P:96:MET:HE2	3:P:220:PRO:HA	1.58	0.85
3:P:111:LEU:CD2	3:P:112:VAL:N	2.37	0.85
3:P:193:GLU:CD	3:P:209:ARG:HH22	1.85	0.85
3:P:415:ILE:HD11	3:P:444:TYR:CE2	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:118:GLY:HA3	3:P:197:PHE:CD2	2.12	0.84
3:P:194:THR:CG2	3:P:195:LEU:H	1.83	0.84
3:P:378:TYR:O	3:P:397:ARG:CB	2.26	0.84
3:P:409:TYR:CE1	3:P:411:GLU:HB2	2.12	0.84
3:P:429:VAL:HG12	3:P:431:LEU:HD11	1.59	0.84
3:P:111:LEU:HD23	3:P:112:VAL:CA	2.09	0.83
3:P:159:GLN:CB	3:P:160:PRO:CD	2.42	0.83
3:P:565:ASN:ND2	3:P:566:ILE:HG13	1.93	0.83
1:N:2:DC:H4'	1:N:3:DA:OP1	1.79	0.83
3:P:137:HIS:HB2	3:P:536:LYS:O	1.78	0.83
3:P:578:LEU:HD23	3:P:578:LEU:H	1.41	0.83
3:P:197:PHE:CE2	3:P:465:PRO:HB2	2.13	0.82
1:N:2:DC:H2'	1:N:2:DC:O2	1.79	0.82
3:P:343:TYR:CE2	3:P:371:ALA:HB1	2.13	0.82
3:P:99:ASP:CG	3:P:216:ARG:HH12	1.85	0.81
2:A:1:DA:H3'	2:A:2:DC:C5'	2.06	0.81
3:P:322:THR:HG21	3:P:420:PHE:CE2	2.16	0.81
3:P:263:THR:HG22	3:P:264:GLY:N	1.93	0.81
3:P:150:LEU:CD2	3:P:525:SER:CB	2.38	0.80
3:P:415:ILE:CD1	3:P:444:TYR:CE2	2.64	0.80
3:P:340:ALA:HB3	3:P:357:ILE:HD11	1.61	0.80
3:P:158:THR:O	3:P:158:THR:CG2	2.30	0.80
3:P:215:ASP:HB3	3:P:234:HIS:HB2	1.62	0.80
3:P:99:ASP:OD1	3:P:216:ARG:NH1	2.14	0.80
3:P:130:VAL:HG13	3:P:578:LEU:HD21	1.59	0.80
3:P:364:ALA:O	3:P:366:THR:N	2.14	0.80
3:P:464:TYR:HA	3:P:465:PRO:O	1.82	0.80
3:P:313:ARG:O	3:P:325:ILE:HD12	1.81	0.80
3:P:86:ASN:ND2	3:P:100:ASP:HB2	1.97	0.80
3:P:465:PRO:HG3	3:P:571:ILE:HG22	1.62	0.80
3:P:415:ILE:HD11	3:P:444:TYR:CD2	2.17	0.80
3:P:122:ASN:HB2	3:P:123:PRO:HD2	1.61	0.79
3:P:51:PHE:CZ	3:P:128:LEU:HD23	2.18	0.79
3:P:193:GLU:OE1	3:P:209:ARG:NH2	2.16	0.79
3:P:494:CYS:HB3	3:P:495:PRO:HD2	1.62	0.79
3:P:276:THR:HG22	3:P:581:ARG:CB	2.12	0.79
3:P:61:ILE:HD11	3:P:133:MET:HE1	1.65	0.79
3:P:93:ASN:HD22	3:P:221:SER:HB2	1.47	0.79
3:P:380:PHE:CD1	3:P:466:ASN:OD1	2.36	0.79
3:P:93:ASN:HD21	3:P:229:PRO:HG3	1.46	0.78
3:P:174:MET:HE3	3:P:504:PRO:CD	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:77:GLU:CG	3:P:520:ARG:NH1	2.46	0.78
3:P:378:TYR:O	3:P:397:ARG:HB3	1.83	0.78
3:P:134:SER:O	3:P:275:LEU:CB	2.31	0.78
3:P:274:ARG:NE	3:P:581:ARG:NH1	2.31	0.78
3:P:469:ILE:HG21	3:P:470:TRP:CE3	2.18	0.78
3:P:52:LYS:HB3	3:P:60:TYR:CB	2.14	0.78
3:P:70:HIS:HD2	3:P:526:ASP:CG	1.93	0.77
3:P:432:PRO:O	3:P:443:ASN:ND2	2.16	0.77
3:P:471:ASP:O	3:P:472:LYS:O	2.01	0.77
3:P:469:ILE:HG22	3:P:470:TRP:HE3	1.50	0.77
3:P:137:HIS:CE1	3:P:272:PRO:HB3	2.19	0.77
3:P:93:ASN:ND2	3:P:229:PRO:HG3	2.00	0.77
3:P:322:THR:HG21	3:P:420:PHE:CD2	2.20	0.77
3:P:490:CYS:C	3:P:490:CYS:CB	2.58	0.77
3:P:373:ASP:OD2	3:P:407:GLY:HA3	1.85	0.76
3:P:464:TYR:CD1	3:P:464:TYR:C	2.64	0.76
3:P:413:ASP:O	3:P:414:TRP:HB3	1.86	0.76
3:P:279:TRP:O	3:P:279:TRP:CE3	2.39	0.76
3:P:415:ILE:CD1	3:P:444:TYR:CD2	2.69	0.76
3:P:46:ASN:HB3	3:P:530:LYS:HE3	1.66	0.75
3:P:217:THR:OG1	3:P:234:HIS:HE1	1.68	0.75
3:P:361:ARG:CD	3:P:405:ASP:OD1	2.34	0.75
3:P:564:SER:O	3:P:567:GLY:N	2.17	0.75
3:P:152:THR:HG23	3:P:521:ILE:HG22	1.68	0.75
3:P:96:MET:CE	3:P:220:PRO:CA	2.65	0.75
3:P:174:MET:CE	3:P:504:PRO:HD2	2.15	0.75
3:P:343:TYR:HE2	3:P:371:ALA:CB	1.99	0.75
3:P:448:PHE:CE2	3:P:450:THR:CG2	2.70	0.75
3:P:68:LEU:HB2	3:P:528:TRP:CE3	2.22	0.75
3:P:66:SER:HA	3:P:530:LYS:HA	1.68	0.74
3:P:146:PHE:HD2	3:P:147:ASN:HD22	1.32	0.74
3:P:150:LEU:HD23	3:P:525:SER:HB3	0.78	0.74
3:P:431:LEU:HB3	3:P:432:PRO:CD	2.16	0.74
3:P:69:VAL:HG13	3:P:205:PRO:HD3	1.68	0.74
3:P:276:THR:O	3:P:577:GLN:NE2	2.21	0.74
3:P:131:ASN:OD1	3:P:550:GLN:HB3	1.88	0.74
3:P:139:VAL:HG12	3:P:140:SER:N	2.02	0.74
3:P:414:TRP:NE1	3:P:416:GLN:HE21	1.86	0.74
3:P:429:VAL:HG12	3:P:431:LEU:HD12	1.69	0.74
3:P:430:LEU:HD21	3:P:436:ILE:HD11	1.70	0.74
3:P:283:ARG:HE	3:P:327:GLU:HB3	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:84:VAL:HG21	3:P:102:HIS:CE1	2.22	0.74
3:P:113:ASP:O	3:P:195:LEU:HD13	1.86	0.74
3:P:533:LEU:CD2	3:P:535:PHE:CZ	2.71	0.74
3:P:138:LEU:HD13	3:P:535:PHE:CE1	2.23	0.74
3:P:111:LEU:HD23	3:P:112:VAL:H	1.52	0.73
3:P:422:LEU:HA	3:P:423:PRO:C	2.12	0.73
3:P:93:ASN:ND2	3:P:221:SER:HB2	2.03	0.73
3:P:429:VAL:CG1	3:P:431:LEU:HD11	2.18	0.73
3:P:111:LEU:HD23	3:P:112:VAL:C	2.12	0.73
3:P:444:TYR:O	3:P:448:PHE:HB2	1.89	0.73
3:P:578:LEU:HD23	3:P:578:LEU:N	2.04	0.73
3:P:68:LEU:HD23	3:P:202:PRO:HB3	1.70	0.73
3:P:424:VAL:HG22	3:P:429:VAL:CG2	1.95	0.72
3:P:533:LEU:HD21	3:P:535:PHE:HZ	1.53	0.72
3:P:47:ASN:ND2	3:P:65:SER:HA	2.05	0.72
3:P:424:VAL:HG11	3:P:429:VAL:HG21	1.71	0.72
3:P:533:LEU:HD21	3:P:535:PHE:CZ	2.25	0.72
3:P:217:THR:O	3:P:231:ASN:HA	1.89	0.72
3:P:368:GLU:O	3:P:369:ASN:HB2	1.88	0.71
3:P:424:VAL:CG1	3:P:429:VAL:HG21	2.19	0.71
3:P:361:ARG:HG2	3:P:405:ASP:OD1	1.91	0.71
3:P:365:GLN:HG2	3:P:401:ILE:HD13	1.72	0.71
3:P:53:PHE:CD1	3:P:59:VAL:CG2	2.74	0.71
3:P:61:ILE:HD11	3:P:133:MET:CE	2.20	0.70
3:P:274:ARG:CD	3:P:581:ARG:HH12	2.03	0.70
3:P:361:ARG:O	3:P:407:GLY:HA3	1.91	0.70
3:P:152:THR:HG23	3:P:521:ILE:CG2	2.21	0.70
3:P:77:GLU:HG2	3:P:520:ARG:HH12	1.53	0.70
3:P:93:ASN:O	3:P:222:HIS:O	2.10	0.69
3:P:414:TRP:CD1	3:P:416:GLN:HE21	2.08	0.69
3:P:465:PRO:CG	3:P:571:ILE:HG22	2.23	0.69
3:P:490:CYS:C	3:P:490:CYS:N	2.48	0.69
3:P:158:THR:O	3:P:158:THR:HG22	1.92	0.69
3:P:274:ARG:NE	3:P:581:ARG:HH11	1.90	0.69
3:P:448:PHE:CE2	3:P:450:THR:HG23	2.28	0.69
3:P:430:LEU:HD11	3:P:436:ILE:HD11	1.75	0.69
3:P:452:GLY:C	3:P:454:LEU:H	2.00	0.69
3:P:53:PHE:HD1	3:P:59:VAL:HG22	1.58	0.69
3:P:64:ASN:HA	3:P:531:GLY:O	1.93	0.69
3:P:482:LEU:N	3:P:482:LEU:HD23	2.08	0.69
3:P:576:SER:O	3:P:578:LEU:CD2	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:378:TYR:CE2	3:P:463:VAL:HG11	2.27	0.68
3:P:109:TRP:CE3	3:P:501:LYS:HB2	2.29	0.68
3:P:158:THR:C	3:P:159:GLN:HG2	2.18	0.68
3:P:157:ALA:CA	3:P:161:PRO:HB3	2.18	0.68
3:P:61:ILE:CD1	3:P:133:MET:HE1	2.23	0.68
3:P:501:LYS:HG2	3:P:502:VAL:N	2.09	0.68
3:P:414:TRP:HE1	3:P:416:GLN:NE2	1.92	0.67
3:P:403:HIS:HD2	3:P:578:LEU:HA	1.58	0.67
3:P:340:ALA:HB1	3:P:341:PRO:HD2	1.75	0.67
3:P:95:ASN:HB3	3:P:98:LEU:HD12	1.77	0.67
3:P:158:THR:C	3:P:160:PRO:HD2	2.16	0.66
3:P:431:LEU:HD12	3:P:431:LEU:N	2.11	0.66
3:P:65:SER:OG	3:P:67:ARG:NH2	2.23	0.66
3:P:390:THR:HG22	3:P:391:THR:N	2.10	0.66
3:P:93:ASN:HD21	3:P:229:PRO:HD3	1.61	0.66
3:P:93:ASN:HD21	3:P:229:PRO:CG	2.09	0.66
3:P:174:MET:CE	3:P:504:PRO:CD	2.73	0.66
3:P:216:ARG:HG2	3:P:232:ILE:O	1.96	0.66
3:P:422:LEU:HB2	3:P:423:PRO:HA	1.78	0.66
3:P:551:MET:HE3	3:P:574:GLU:CD	2.21	0.65
3:P:55:GLU:O	3:P:56:ASN:HB2	1.96	0.65
3:P:426:ASN:C	3:P:428:ASN:H	2.04	0.65
3:P:126:TRP:O	3:P:130:VAL:HG23	1.96	0.65
3:P:361:ARG:CG	3:P:405:ASP:OD1	2.44	0.65
1:N:3:DA:H5'	1:N:9:DA:C5'	2.26	0.65
3:P:274:ARG:CZ	3:P:581:ARG:NH1	2.59	0.65
1:N:2:DC:O2	1:N:2:DC:C2'	2.43	0.65
3:P:115:ASN:OD1	3:P:469:ILE:HB	1.97	0.65
3:P:370:GLN:NE2	3:P:399:THR:HG21	2.10	0.65
3:P:155:GLU:OE2	3:P:163:LYS:HE2	1.97	0.64
3:P:322:THR:CG2	3:P:420:PHE:HD2	2.07	0.64
3:P:51:PHE:CE1	3:P:128:LEU:HD23	2.33	0.64
3:P:469:ILE:HG22	3:P:470:TRP:CE3	2.27	0.64
3:P:564:SER:O	3:P:566:ILE:N	2.30	0.64
3:P:417:ASN:HB2	3:P:428:ASN:HD22	1.63	0.64
3:P:109:TRP:CZ3	3:P:501:LYS:HB3	2.32	0.63
3:P:343:TYR:CE2	3:P:371:ALA:CB	2.77	0.63
3:P:174:MET:HE3	3:P:504:PRO:HD3	1.80	0.63
3:P:274:ARG:CZ	3:P:581:ARG:HH11	2.11	0.63
3:P:66:SER:HB3	3:P:530:LYS:HG3	1.81	0.63
3:P:469:ILE:HG21	3:P:470:TRP:HE3	1.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:183:MET:HG2	3:P:208:TRP:HH2	1.63	0.63
3:P:370:GLN:HA	3:P:375:ASN:OD1	1.98	0.63
3:P:414:TRP:HE1	3:P:416:GLN:HE21	1.47	0.63
3:P:160:PRO:CB	3:P:161:PRO:C	2.65	0.62
3:P:245:THR:O	3:P:249:SER:OG	2.16	0.62
3:P:471:ASP:C	3:P:472:LYS:O	2.42	0.62
3:P:107:THR:OG1	3:P:208:TRP:HB3	1.99	0.62
3:P:313:ARG:O	3:P:325:ILE:CD1	2.45	0.62
3:P:270:CYS:HB3	3:P:490:CYS:HA	1.82	0.62
3:P:508:ASN:ND2	3:P:509:GLN:HG3	2.15	0.62
3:P:409:TYR:C	3:P:411:GLU:H	2.08	0.62
3:P:279:TRP:CE3	3:P:279:TRP:C	2.78	0.62
3:P:341:PRO:HB2	3:P:344:SER:HB2	1.82	0.62
3:P:533:LEU:HG	3:P:535:PHE:CE2	2.34	0.62
3:P:75:GLU:HG3	3:P:76:SER:HB2	1.82	0.62
3:P:116:ALA:O	3:P:120:TRP:HD1	1.83	0.62
3:P:174:MET:HE3	3:P:503:ALA:CA	2.20	0.62
3:P:183:MET:CG	3:P:184:PRO:HD2	2.30	0.62
3:P:326:THR:H	3:P:329:THR:HB	1.64	0.62
3:P:96:MET:HE1	3:P:221:SER:N	1.94	0.62
3:P:500:VAL:HG11	3:P:527:PHE:CZ	2.35	0.62
3:P:390:THR:HG22	3:P:391:THR:H	1.65	0.61
3:P:443:ASN:HB3	3:P:445:THR:H	1.65	0.61
3:P:122:ASN:ND2	3:P:125:ASP:CG	2.59	0.61
3:P:37:GLY:O	3:P:39:GLY:N	2.26	0.61
3:P:232:ILE:HG22	3:P:233:TYR:N	2.16	0.61
3:P:180:ASN:O	3:P:181:ASN:C	2.44	0.61
3:P:70:HIS:CG	3:P:526:ASP:OD2	2.50	0.60
3:P:88:ASP:OD1	3:P:89:LYS:HG2	2.00	0.60
3:P:138:LEU:CD1	3:P:535:PHE:CE1	2.83	0.60
3:P:216:ARG:CG	3:P:232:ILE:O	2.50	0.60
3:P:459:ASN:HA	3:P:482:LEU:HD12	1.83	0.60
3:P:385:GLY:O	3:P:386:GLN:O	2.19	0.60
3:P:482:LEU:HD23	3:P:482:LEU:H	1.66	0.60
3:P:533:LEU:CD2	3:P:535:PHE:HZ	2.11	0.60
3:P:174:MET:HE3	3:P:504:PRO:HD2	1.76	0.60
3:P:219:ILE:HG13	3:P:230:THR:CB	2.28	0.60
3:P:317:THR:HG23	3:P:329:THR:HG22	1.84	0.60
3:P:75:GLU:C	3:P:520:ARG:HH22	2.09	0.60
3:P:93:ASN:HD21	3:P:229:PRO:CD	2.15	0.60
3:P:122:ASN:HD21	3:P:125:ASP:CG	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:203:THR:OG1	3:P:204:ILE:N	2.32	0.60
3:P:292:ASN:HB2	3:P:306:ILE:O	2.02	0.60
3:P:197:PHE:HE2	3:P:465:PRO:CB	2.12	0.59
3:P:276:THR:HG22	3:P:581:ARG:HB3	1.83	0.59
3:P:578:LEU:O	3:P:578:LEU:HG	2.02	0.59
3:P:111:LEU:CD2	3:P:112:VAL:C	2.75	0.59
3:P:361:ARG:HG3	3:P:362:GLY:N	2.14	0.59
3:P:368:GLU:HB2	3:P:370:GLN:H	1.68	0.59
3:P:80:ARG:O	3:P:105:ILE:HG23	2.02	0.59
3:P:56:ASN:O	3:P:58:TRP:CD1	2.56	0.59
3:P:152:THR:CG2	3:P:521:ILE:CG2	2.80	0.59
3:P:322:THR:HG22	3:P:420:PHE:HD2	1.68	0.59
2:A:1:DA:C2'	2:A:2:DC:O4'	2.42	0.58
3:P:160:PRO:HG2	3:P:162:THR:OG1	2.04	0.58
3:P:557:ASN:O	3:P:560:ASN:HB2	2.02	0.58
3:P:364:ALA:O	3:P:367:ASP:N	2.36	0.58
3:P:422:LEU:CA	3:P:423:PRO:C	2.75	0.58
3:P:465:PRO:CG	3:P:571:ILE:CG2	2.73	0.58
3:P:111:LEU:O	3:P:205:PRO:CB	2.52	0.58
3:P:448:PHE:CE2	3:P:450:THR:HG21	2.37	0.58
3:P:343:TYR:HE2	3:P:371:ALA:HB1	1.56	0.58
3:P:517:ASN:C	3:P:518:MET:O	2.47	0.58
3:P:198:TYR:OH	3:P:570:LYS:HA	2.03	0.58
3:P:562:VAL:HG13	3:P:563:PRO:HD2	1.85	0.58
3:P:70:HIS:CD2	3:P:526:ASP:CG	2.74	0.58
3:P:274:ARG:CD	3:P:581:ARG:NH1	2.66	0.58
3:P:75:GLU:HG3	3:P:76:SER:CB	2.33	0.57
3:P:420:PHE:O	3:P:421:ASN:C	2.47	0.57
3:P:77:GLU:CG	3:P:520:ARG:HH11	2.17	0.57
3:P:324:TYR:O	3:P:329:THR:HG21	2.05	0.57
3:P:339:SER:HB2	3:P:450:THR:OG1	2.04	0.57
3:P:73:MET:CE	3:P:520:ARG:CG	2.80	0.57
3:P:285:LEU:HD22	3:P:584:TYR:HB3	1.86	0.57
3:P:93:ASN:ND2	3:P:221:SER:CB	2.66	0.57
3:P:415:ILE:HD12	3:P:444:TYR:CD2	2.38	0.57
3:P:84:VAL:O	3:P:101:ILE:HG13	2.03	0.57
3:P:111:LEU:O	3:P:205:PRO:HB3	2.04	0.57
3:P:188:ALA:HB1	3:P:193:GLU:O	2.05	0.57
3:P:115:ASN:ND2	3:P:470:TRP:O	2.30	0.57
3:P:354:LYS:HD2	3:P:355:THR:N	2.19	0.57
3:P:140:SER:H	3:P:534:VAL:HB	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:243:PHE:CD1	3:P:243:PHE:C	2.82	0.57
3:P:447:ILE:O	3:P:447:ILE:HG22	2.05	0.57
3:P:47:ASN:HD22	3:P:66:SER:H	1.53	0.56
3:P:136:LEU:HD12	3:P:537:ALA:HB2	1.86	0.56
3:P:142:GLU:HB2	3:P:264:GLY:O	2.03	0.56
3:P:122:ASN:HB2	3:P:123:PRO:CD	2.34	0.56
3:P:142:GLU:CB	3:P:264:GLY:O	2.53	0.56
3:P:247:GLU:CD	3:P:247:GLU:H	2.13	0.56
3:P:77:GLU:OE2	3:P:520:ARG:NH1	2.39	0.56
3:P:219:ILE:CG1	3:P:230:THR:HB	2.29	0.56
3:P:109:TRP:CE3	3:P:501:LYS:CB	2.89	0.56
3:P:117:TRP:CZ2	3:P:462:PRO:HB3	2.41	0.56
3:P:68:LEU:HB2	3:P:528:TRP:CZ3	2.41	0.56
3:P:93:ASN:O	3:P:221:SER:O	2.23	0.56
3:P:111:LEU:HD23	3:P:111:LEU:C	2.27	0.56
3:P:86:ASN:CG	3:P:86:ASN:O	2.49	0.56
3:P:96:MET:CE	3:P:220:PRO:CB	2.84	0.56
3:P:110:SER:HB2	3:P:500:VAL:O	2.05	0.56
3:P:548:ILE:HG23	3:P:580:PRO:CD	2.36	0.55
3:P:132:THR:O	3:P:540:ARG:HG2	2.06	0.55
3:P:361:ARG:HD3	3:P:405:ASP:OD1	2.05	0.55
3:P:365:GLN:HG2	3:P:401:ILE:CD1	2.35	0.55
3:P:426:ASN:O	3:P:428:ASN:N	2.39	0.55
3:P:73:MET:HE3	3:P:520:ARG:CD	2.37	0.55
3:P:73:MET:HE3	3:P:520:ARG:HE	1.71	0.55
3:P:75:GLU:HG3	3:P:76:SER:CA	2.32	0.55
3:P:452:GLY:C	3:P:454:LEU:N	2.64	0.55
3:P:461:PRO:HB3	3:P:577:GLN:OE1	2.07	0.55
3:P:578:LEU:CD2	3:P:578:LEU:N	2.69	0.55
3:P:96:MET:CE	3:P:220:PRO:HA	2.31	0.55
3:P:419:ASN:O	3:P:421:ASN:N	2.37	0.55
3:P:548:ILE:HG23	3:P:580:PRO:HD2	1.88	0.55
3:P:326:THR:HG22	3:P:327:GLU:N	2.22	0.55
3:P:409:TYR:O	3:P:411:GLU:N	2.40	0.55
3:P:96:MET:HE1	3:P:220:PRO:CB	2.37	0.54
3:P:373:ASP:OD2	3:P:407:GLY:CA	2.54	0.54
3:P:130:VAL:HG13	3:P:578:LEU:CD2	2.27	0.54
3:P:381:GLY:CA	3:P:386:GLN:NE2	2.59	0.54
3:P:96:MET:CE	3:P:220:PRO:C	2.62	0.54
3:P:194:THR:HB	3:P:384:HIS:CE1	2.42	0.54
3:P:255:LEU:HD13	3:P:259:ASP:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:472:LYS:HG2	3:P:473:GLU:H	1.72	0.54
3:P:377:ARG:CZ	3:P:397:ARG:HG3	2.38	0.54
3:P:501:LYS:CG	3:P:502:VAL:N	2.71	0.54
3:P:47:ASN:HA	3:P:64:ASN:O	2.07	0.54
3:P:482:LEU:N	3:P:482:LEU:CD2	2.71	0.54
3:P:57:GLY:O	3:P:539:LEU:HG	2.08	0.54
3:P:426:ASN:C	3:P:428:ASN:N	2.64	0.54
3:P:339:SER:O	3:P:449:ASN:HA	2.07	0.54
3:P:177:LEU:O	3:P:250:VAL:HG13	2.08	0.53
3:P:77:GLU:CD	3:P:520:ARG:NH1	2.67	0.53
1:N:4:DC:H3'	1:N:5:DC:H5'	1.89	0.53
3:P:538:LYS:HG3	3:P:539:LEU:N	2.23	0.53
3:P:557:ASN:HB3	3:P:561:TYR:HE2	1.74	0.53
3:P:110:SER:O	3:P:500:VAL:O	2.27	0.53
3:P:313:ARG:C	3:P:325:ILE:HD12	2.33	0.52
3:P:422:LEU:HA	3:P:424:VAL:N	2.23	0.52
3:P:459:ASN:HD22	3:P:482:LEU:HB2	1.74	0.52
3:P:136:LEU:HD11	3:P:535:PHE:HB3	1.89	0.52
3:P:494:CYS:HB3	3:P:495:PRO:CD	2.35	0.52
3:P:193:GLU:HB3	3:P:206:THR:HG22	1.86	0.52
3:P:432:PRO:HA	3:P:443:ASN:ND2	2.24	0.52
3:P:232:ILE:CG2	3:P:233:TYR:N	2.73	0.52
3:P:343:TYR:HE2	3:P:371:ALA:HB2	1.73	0.52
3:P:576:SER:O	3:P:578:LEU:HD22	2.08	0.52
3:P:468:GLN:OE1	3:P:471:ASP:HB2	2.10	0.52
3:P:103:ALA:HB3	3:P:212:PHE:O	2.10	0.52
3:P:197:PHE:CE2	3:P:465:PRO:CB	2.89	0.52
3:P:443:ASN:CB	3:P:445:THR:OG1	2.58	0.51
3:P:136:LEU:HA	3:P:537:ALA:HB2	1.91	0.51
3:P:158:THR:H	3:P:161:PRO:HB3	1.76	0.51
3:P:57:GLY:HA2	3:P:539:LEU:HD12	1.93	0.51
3:P:183:MET:HG2	3:P:184:PRO:HD2	1.92	0.51
3:P:390:THR:CG2	3:P:391:THR:H	2.23	0.51
3:P:111:LEU:CD2	3:P:112:VAL:H	2.14	0.50
3:P:299:GLY:C	3:P:301:THR:H	2.19	0.50
3:P:413:ASP:O	3:P:414:TRP:CB	2.59	0.50
3:P:541:ALA:HB3	3:P:543:HIS:CE1	2.47	0.50
3:P:554:ASN:HB2	3:P:557:ASN:HD22	1.76	0.50
3:P:37:GLY:C	3:P:39:GLY:H	2.16	0.50
3:P:45:PHE:HE1	3:P:47:ASN:HB2	1.76	0.50
3:P:365:GLN:OE1	3:P:365:GLN:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:390:THR:CG2	3:P:391:THR:N	2.74	0.50
3:P:137:HIS:CB	3:P:536:LYS:O	2.57	0.50
3:P:113:ASP:OD2	3:P:188:ALA:N	2.43	0.50
3:P:466:ASN:O	3:P:467:GLY:C	2.53	0.50
3:P:139:VAL:CG1	3:P:140:SER:N	2.69	0.50
3:P:338:TYR:CE1	3:P:357:ILE:HD13	2.47	0.50
3:P:410:PRO:HA	3:P:413:ASP:OD1	2.11	0.50
3:P:417:ASN:CB	3:P:428:ASN:HD22	2.25	0.49
3:P:459:ASN:CG	3:P:460:VAL:N	2.70	0.49
3:P:216:ARG:HG2	3:P:217:THR:H	1.77	0.49
3:P:224:GLY:O	3:P:225:THR:C	2.55	0.49
3:P:73:MET:HB2	3:P:523:THR:O	2.12	0.49
3:P:158:THR:O	3:P:158:THR:HG23	2.10	0.49
3:P:101:ILE:O	3:P:101:ILE:HG23	2.10	0.49
3:P:382:ARG:HG2	3:P:382:ARG:HH11	1.77	0.49
3:P:471:ASP:O	3:P:472:LYS:C	2.55	0.49
3:P:160:PRO:HG2	3:P:161:PRO:C	2.37	0.49
3:P:160:PRO:CG	3:P:161:PRO:C	2.86	0.49
3:P:116:ALA:O	3:P:120:TRP:CD1	2.64	0.49
3:P:414:TRP:NE1	3:P:416:GLN:NE2	2.53	0.49
3:P:125:ASP:O	3:P:128:LEU:HB3	2.12	0.49
3:P:199:PRO:C	3:P:201:LYS:H	2.20	0.49
3:P:564:SER:C	3:P:566:ILE:N	2.71	0.49
3:P:75:GLU:HG2	3:P:76:SER:N	1.92	0.48
3:P:403:HIS:NE2	3:P:549:GLN:NE2	2.61	0.48
3:P:463:VAL:O	3:P:465:PRO:O	2.31	0.48
3:P:96:MET:HE3	3:P:221:SER:C	2.38	0.48
3:P:109:TRP:CG	3:P:246:ILE:HD12	2.48	0.48
3:P:282:ASN:O	3:P:332:ARG:NE	2.46	0.48
3:P:435:PRO:HB3	3:P:439:LYS:O	2.12	0.48
3:P:65:SER:O	3:P:529:TRP:CZ3	2.67	0.48
3:P:137:HIS:ND1	3:P:272:PRO:HB3	2.28	0.48
3:P:198:TYR:CE1	3:P:571:ILE:HG13	2.48	0.48
3:P:219:ILE:HG22	3:P:220:PRO:HD2	1.95	0.48
3:P:576:SER:OG	3:P:577:GLN:N	2.46	0.48
3:P:67:ARG:N	3:P:529:TRP:O	2.46	0.48
3:P:510:TYR:HE1	3:P:518:MET:HG2	1.79	0.48
3:P:545:TRP:CD1	3:P:545:TRP:C	2.91	0.48
3:P:551:MET:HE3	3:P:574:GLU:OE2	2.12	0.48
3:P:472:LYS:HG2	3:P:473:GLU:N	2.29	0.48
3:P:442:ILE:HG22	3:P:443:ASN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:111:LEU:CG	3:P:112:VAL:N	2.77	0.47
3:P:431:LEU:CD1	3:P:431:LEU:N	2.75	0.47
3:P:432:PRO:HA	3:P:443:ASN:HD22	1.79	0.47
3:P:565:ASN:HD21	3:P:566:ILE:HG13	1.76	0.47
3:P:53:PHE:CE1	3:P:59:VAL:CG2	2.98	0.47
3:P:184:PRO:HD3	3:P:244:TYR:CE2	2.49	0.47
3:P:53:PHE:CE1	3:P:59:VAL:HG21	2.50	0.47
3:P:93:ASN:O	3:P:222:HIS:C	2.57	0.47
3:P:360:GLY:HA3	3:P:404:GLN:HG3	1.97	0.47
3:P:45:PHE:CD1	3:P:45:PHE:C	2.92	0.47
3:P:408:ARG:O	3:P:410:PRO:HD3	2.15	0.47
3:P:430:LEU:HD21	3:P:436:ILE:CD1	2.42	0.47
3:P:391:THR:HG22	3:P:392:GLY:N	2.30	0.47
3:P:469:ILE:HG22	3:P:470:TRP:N	2.29	0.47
3:P:221:SER:CB	3:P:229:PRO:HG3	2.45	0.46
3:P:381:GLY:HA2	3:P:386:GLN:HE22	1.72	0.46
3:P:93:ASN:C	3:P:221:SER:O	2.58	0.46
3:P:140:SER:HA	3:P:266:PHE:O	2.15	0.46
3:P:158:THR:N	3:P:161:PRO:HB3	2.31	0.46
3:P:103:ALA:CB	3:P:214:TRP:HB3	2.44	0.46
3:P:291:LEU:CD2	3:P:306:ILE:HG12	2.46	0.46
3:P:373:ASP:O	3:P:374:GLY:C	2.57	0.46
3:P:557:ASN:O	3:P:558:GLN:C	2.57	0.46
3:P:255:LEU:CD1	3:P:259:ASP:HB3	2.45	0.46
3:P:283:ARG:HD2	3:P:327:GLU:O	2.14	0.46
3:P:95:ASN:CB	3:P:98:LEU:HD12	2.45	0.46
3:P:283:ARG:NE	3:P:327:GLU:HB3	2.26	0.46
3:P:46:ASN:C	3:P:66:SER:HG	2.23	0.46
3:P:400:TYR:OH	3:P:575:LYS:HA	2.15	0.46
3:P:422:LEU:HB2	3:P:423:PRO:CA	2.45	0.46
3:P:378:TYR:O	3:P:397:ARG:HB2	2.14	0.46
3:P:380:PHE:CE1	3:P:398:PHE:CE1	3.04	0.46
3:P:557:ASN:O	3:P:560:ASN:N	2.48	0.46
3:P:151:LYS:HE2	3:P:167:ASN:OD1	2.16	0.46
3:P:286:GLY:O	3:P:288:PRO:HD3	2.16	0.46
3:P:576:SER:O	3:P:578:LEU:HD23	2.16	0.46
3:P:408:ARG:C	3:P:410:PRO:HD3	2.41	0.46
3:P:540:ARG:HG3	3:P:540:ARG:O	2.16	0.45
3:P:572:VAL:HG12	3:P:573:TYR:O	2.16	0.45
3:P:62:THR:HG21	3:P:532:LYS:HE3	1.98	0.45
3:P:73:MET:HE3	3:P:520:ARG:CG	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:473:GLU:OE2	3:P:489:VAL:HG11	2.16	0.45
3:P:551:MET:CE	3:P:574:GLU:OE1	2.64	0.45
3:P:67:ARG:NH1	3:P:196:GLY:O	2.50	0.45
3:P:103:ALA:HB3	3:P:214:TRP:HB3	1.98	0.45
3:P:443:ASN:HB3	3:P:445:THR:OG1	2.17	0.45
3:P:216:ARG:HG2	3:P:217:THR:N	2.32	0.45
3:P:183:MET:HE2	3:P:244:TYR:HB3	1.99	0.45
3:P:383:GLN:O	3:P:383:GLN:HG2	2.16	0.45
3:P:109:TRP:CD1	3:P:246:ILE:HD12	2.51	0.45
3:P:174:MET:CE	3:P:504:PRO:HD3	2.43	0.45
3:P:237:ASP:C	3:P:239:ASP:H	2.23	0.45
3:P:365:GLN:C	3:P:365:GLN:CD	2.84	0.45
3:P:383:GLN:C	3:P:384:HIS:CD2	2.95	0.45
3:P:387:LYS:HA	3:P:570:LYS:HB3	1.98	0.45
3:P:551:MET:HE3	3:P:574:GLU:OE1	2.16	0.45
3:P:150:LEU:HD21	3:P:525:SER:CB	2.38	0.45
3:P:45:PHE:CD1	3:P:46:ASN:N	2.86	0.44
3:P:191:ARG:O	3:P:193:GLU:HG3	2.17	0.44
3:P:533:LEU:CD2	3:P:535:PHE:CE2	2.99	0.44
3:P:93:ASN:ND2	3:P:229:PRO:CG	2.74	0.44
3:P:135:GLU:O	3:P:537:ALA:HB1	2.17	0.44
3:P:138:LEU:HD11	3:P:533:LEU:HD11	1.98	0.44
3:P:391:THR:CG2	3:P:392:GLY:N	2.81	0.44
3:P:505:ASN:O	3:P:520:ARG:HB2	2.18	0.44
3:P:552:SER:OG	3:P:553:ILE:N	2.51	0.44
3:P:117:TRP:HZ2	3:P:487:PRO:HG2	1.81	0.44
3:P:221:SER:HB3	3:P:229:PRO:HG3	1.99	0.44
3:P:325:ILE:HG23	3:P:330:ILE:HG12	1.99	0.44
3:P:158:THR:O	3:P:159:GLN:CB	2.65	0.44
3:P:317:THR:HG22	3:P:318:GLN:N	2.33	0.44
3:P:382:ARG:H	3:P:386:GLN:HB3	1.82	0.44
3:P:474:PHE:CD1	3:P:474:PHE:N	2.85	0.44
3:P:422:LEU:HB2	3:P:424:VAL:N	2.32	0.43
3:P:140:SER:HB2	3:P:534:VAL:CG2	2.47	0.43
3:P:175:VAL:HG23	3:P:255:LEU:HD23	2.00	0.43
3:P:448:PHE:CZ	3:P:450:THR:CG2	3.01	0.43
3:P:470:TRP:HA	3:P:488:PHE:O	2.19	0.43
3:P:80:ARG:O	3:P:105:ILE:HA	2.19	0.43
3:P:422:LEU:HB2	3:P:424:VAL:H	1.82	0.43
3:P:217:THR:OG1	3:P:234:HIS:CE1	2.59	0.43
3:P:413:ASP:C	3:P:414:TRP:HE3	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:572:VAL:HG12	3:P:573:TYR:N	2.34	0.43
3:P:130:VAL:HG11	3:P:578:LEU:HD21	1.79	0.43
3:P:134:SER:OG	3:P:135:GLU:N	2.51	0.43
3:P:383:GLN:HB3	3:P:384:HIS:CD2	2.53	0.43
3:P:71:LEU:HD21	3:P:502:VAL:HG23	2.01	0.43
3:P:181:ASN:HD22	3:P:493:ASN:HD21	1.67	0.43
3:P:183:MET:HG2	3:P:208:TRP:CH2	2.50	0.43
3:P:68:LEU:HB2	3:P:528:TRP:CD2	2.54	0.43
3:P:346:GLU:O	3:P:352:PRO:HA	2.19	0.43
3:P:122:ASN:ND2	3:P:125:ASP:H	2.16	0.42
3:P:130:VAL:HG13	3:P:576:SER:O	2.19	0.42
3:P:334:ALA:HB1	3:P:454:LEU:O	2.19	0.42
3:P:71:LEU:HD12	3:P:72:ASN:N	2.35	0.42
3:P:110:SER:O	3:P:500:VAL:N	2.50	0.42
3:P:111:LEU:CG	3:P:112:VAL:H	2.32	0.42
3:P:138:LEU:HD13	3:P:535:PHE:HE1	1.78	0.42
3:P:158:THR:HG23	3:P:159:GLN:HG2	2.01	0.42
3:P:364:ALA:C	3:P:366:THR:N	2.76	0.42
3:P:403:HIS:CD2	3:P:577:GLN:O	2.72	0.42
3:P:490:CYS:C	3:P:490:CYS:HB2	2.42	0.42
3:P:139:VAL:O	3:P:268:PHE:HB2	2.20	0.42
3:P:196:GLY:HA2	3:P:383:GLN:HG2	2.00	0.42
3:P:263:THR:CG2	3:P:264:GLY:N	2.60	0.42
3:P:45:PHE:HD1	3:P:46:ASN:N	2.17	0.42
3:P:219:ILE:CD1	3:P:230:THR:HB	2.50	0.42
3:P:425:THR:O	3:P:428:ASN:HB2	2.19	0.42
3:P:564:SER:C	3:P:566:ILE:H	2.27	0.42
2:A:1:DA:H2'	2:A:2:DC:H5''	1.74	0.42
3:P:86:ASN:O	3:P:86:ASN:OD1	2.37	0.42
3:P:177:LEU:O	3:P:250:VAL:CG1	2.67	0.42
3:P:361:ARG:NE	3:P:405:ASP:OD1	2.52	0.42
3:P:368:GLU:HB2	3:P:369:ASN:H	1.11	0.42
3:P:378:TYR:O	3:P:397:ARG:CA	2.67	0.42
3:P:415:ILE:HG13	3:P:444:TYR:CE2	2.55	0.42
3:P:84:VAL:O	3:P:101:ILE:HA	2.19	0.42
3:P:178:ASP:OD2	3:P:181:ASN:HA	2.20	0.42
3:P:247:GLU:CD	3:P:247:GLU:N	2.76	0.42
3:P:462:PRO:O	3:P:576:SER:HB3	2.20	0.42
1:N:9:DA:H2'	1:N:9:DA:N3	2.35	0.41
3:P:340:ALA:HB1	3:P:341:PRO:CD	2.48	0.41
3:P:162:THR:HG22	3:P:163:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:347:ALA:HB2	3:P:352:PRO:HA	2.01	0.41
3:P:366:THR:O	3:P:366:THR:CG2	2.68	0.41
3:P:45:PHE:C	3:P:45:PHE:HD1	2.27	0.41
3:P:85:ASN:HD21	3:P:87:MET:HE2	1.86	0.41
3:P:139:VAL:O	3:P:268:PHE:HD2	2.03	0.41
3:P:548:ILE:HG23	3:P:580:PRO:HD3	2.03	0.41
3:P:44:THR:HG22	3:P:45:PHE:N	2.35	0.41
3:P:131:ASN:ND2	3:P:551:MET:HB3	2.19	0.41
3:P:440:THR:O	3:P:442:ILE:N	2.53	0.41
3:P:101:ILE:O	3:P:101:ILE:CG2	2.68	0.41
3:P:213:GLN:HG3	3:P:240:ASP:HB2	2.02	0.41
3:P:465:PRO:HB2	3:P:466:ASN:H	1.64	0.41
3:P:197:PHE:HB3	3:P:571:ILE:HD12	2.02	0.41
3:P:47:ASN:HD22	3:P:66:SER:N	2.17	0.41
3:P:59:VAL:CG1	3:P:60:TYR:N	2.84	0.41
3:P:59:VAL:HG12	3:P:60:TYR:N	2.35	0.41
3:P:93:ASN:ND2	3:P:229:PRO:HD3	2.34	0.41
3:P:160:PRO:CG	3:P:161:PRO:O	2.62	0.41
3:P:237:ASP:C	3:P:239:ASP:N	2.79	0.41
3:P:309:GLN:O	3:P:313:ARG:HG3	2.21	0.41
3:P:68:LEU:CD2	3:P:202:PRO:HB3	2.47	0.41
3:P:68:LEU:HD13	3:P:528:TRP:CE2	2.56	0.41
3:P:91:ALA:C	3:P:93:ASN:N	2.78	0.41
3:P:452:GLY:O	3:P:454:LEU:N	2.54	0.41
3:P:62:THR:CG2	3:P:532:LYS:HE3	2.51	0.40
3:P:301:THR:O	3:P:303:PHE:CE2	2.75	0.40
3:P:326:THR:O	3:P:330:ILE:HG13	2.20	0.40
3:P:432:PRO:C	3:P:443:ASN:HD21	2.29	0.40
3:P:176:ALA:HB3	3:P:499:PHE:HB2	2.03	0.40
3:P:214:TRP:NE1	3:P:350:GLN:O	2.53	0.40
3:P:380:PHE:HE1	3:P:398:PHE:CE1	2.39	0.40
3:P:187:PRO:HB2	3:P:468:GLN:NE2	2.36	0.40
3:P:430:LEU:CD2	3:P:436:ILE:HD11	2.46	0.40
3:P:464:TYR:CD1	3:P:465:PRO:N	2.89	0.40
3:P:562:VAL:CG1	3:P:563:PRO:HD2	2.49	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
3	P	546/584 (94%)	442 (81%)	70 (13%)	34 (6%)	1 7

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	38	VAL
3	P	159	GLN
3	P	369	ASN
3	P	370	GLN
3	P	386	GLN
3	P	402	ALA
3	P	465	PRO
3	P	466	ASN
3	P	467	GLY
3	P	472	LYS
3	P	518	MET
3	P	558	GLN
3	P	565	ASN
3	P	56	ASN
3	P	157	ALA
3	P	229	PRO
3	P	360	GLY
3	P	365	GLN
3	P	366	THR
3	P	374	GLY
3	P	427	ASP
3	P	522	VAL
3	P	181	ASN
3	P	221	SER
3	P	421	ASN
3	P	441	GLY
3	P	230	THR
3	P	225	THR

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Mol	Chain	Res	Type
3	P	414	TRP
3	P	420	PHE
3	P	426	ASN
3	P	410	PRO
3	P	453	PRO
3	P	94	GLY

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	P	477/496 (96%)	427 (90%)	50 (10%)	6 24

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	38	VAL
3	P	41	SER
3	P	42	THR
3	P	47	ASN
3	P	48	GLN
3	P	65	SER
3	P	66	SER
3	P	67	ARG
3	P	68	LEU
3	P	71	LEU
3	P	78	ASN
3	P	81	ARG
3	P	87	MET
3	P	92	VAL
3	P	96	MET
3	P	122	ASN
3	P	158	THR
3	P	170	THR
3	P	173	LEU
3	P	177	LEU

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Mol	Chain	Res	Type
3	P	180	ASN
3	P	183	MET
3	P	191	ARG
3	P	203	THR
3	P	208	TRP
3	P	213	GLN
3	P	215	ASP
3	P	219	ILE
3	P	230	THR
3	P	231	ASN
3	P	240	ASP
3	P	249	SER
3	P	349	THR
3	P	354	LYS
3	P	355	THR
3	P	357	ILE
3	P	365	GLN
3	P	366	THR
3	P	367	ASP
3	P	368	GLU
3	P	387	LYS
3	P	393	GLU
3	P	417	ASN
3	P	420	PHE
3	P	422	LEU
3	P	464	TYR
3	P	482	LEU
3	P	490	CYS
3	P	518	MET
3	P	578	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
3	P	47	ASN
3	P	48	GLN
3	P	56	ASN
3	P	64	ASN
3	P	70	HIS
3	P	85	ASN
3	P	93	ASN
3	P	122	ASN

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Mol	Chain	Res	Type
3	P	137	HIS
3	P	147	ASN
3	P	180	ASN
3	P	181	ASN
3	P	234	HIS
3	P	282	ASN
3	P	292	ASN
3	P	302	ASN
3	P	370	GLN
3	P	384	HIS
3	P	386	GLN
3	P	403	HIS
3	P	416	GLN
3	P	428	ASN
3	P	443	ASN
3	P	459	ASN
3	P	492	ASN
3	P	508	ASN
3	P	517	ASN
3	P	543	HIS
3	P	549	GLN
3	P	557	ASN
3	P	565	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	239:ASP	C	240:ASP	N	1.15

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	N	9/9 (100%)	1.33	3 (33%) 1 1	12, 12, 12, 12	0
2	A	2/2 (100%)	0.54	0 100 100	12, 12, 12, 12	0
3	P	548/584 (93%)	1.07	90 (16%) 4 4	0, 12, 12, 15	0
All	All	559/595 (93%)	1.07	93 (16%) 4 4	0, 12, 12, 15	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	340	ALA	9.6
3	P	257	THR	5.7
3	P	223	THR	5.4
3	P	91	ALA	4.8
3	P	97	ALA	4.3
3	P	85	ASN	4.2
3	P	245	THR	3.8
3	P	140	SER	3.7
3	P	47	ASN	3.6
3	P	180	ASN	3.6
3	P	281	THR	3.5
3	P	106	VAL	3.5
3	P	484	VAL	3.5
3	P	481	ARG	3.4
3	P	229	PRO	3.4
3	P	224	GLY	3.3
3	P	120	TRP	3.3
3	P	466	ASN	3.3
3	P	109	TRP	3.3
3	P	144	GLU	3.3
3	P	258	GLY	3.3
3	P	297	SER	3.2
3	P	46	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
3	P	453	PRO	3.2
3	P	278	THR	3.1
3	P	436	ILE	3.1
3	P	94	GLY	3.0
3	P	417	ASN	3.0
3	P	239	ASP	3.0
1	N	4	DC	2.9
3	P	87	MET	2.9
3	P	191	ARG	2.8
3	P	182	THR	2.8
3	P	248	ASN	2.8
3	P	195	LEU	2.8
3	P	305	ASP	2.7
3	P	116	ALA	2.7
3	P	316	VAL	2.7
3	P	263	THR	2.7
3	P	238	PRO	2.6
3	P	497	GLN	2.6
1	N	3	DA	2.6
3	P	250	VAL	2.6
3	P	77	GLU	2.5
3	P	450	THR	2.5
1	N	1	DC	2.5
3	P	402	ALA	2.5
3	P	260	GLU	2.5
3	P	551	MET	2.5
3	P	556	ASP	2.5
3	P	359	ALA	2.4
3	P	179	SER	2.4
3	P	525	SER	2.4
3	P	81	ARG	2.4
3	P	550	GLN	2.4
3	P	409	TYR	2.4
3	P	412	GLY	2.4
3	P	215	ASP	2.4
3	P	363	GLY	2.4
3	P	247	GLU	2.4
3	P	232	ILE	2.3
3	P	560	ASN	2.3
3	P	362	GLY	2.3
3	P	358	ALA	2.3
3	P	507	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	P	422	LEU	2.3
3	P	212	PHE	2.3
3	P	71	LEU	2.2
3	P	118	GLY	2.2
3	P	128	LEU	2.2
3	P	236	THR	2.2
3	P	485	ASN	2.2
3	P	168	ASP	2.2
3	P	103	ALA	2.2
3	P	235	GLY	2.2
3	P	330	ILE	2.2
3	P	328	ALA	2.1
3	P	355	THR	2.1
3	P	524	TYR	2.1
3	P	284	ALA	2.1
3	P	471	ASP	2.1
3	P	43	GLY	2.1
3	P	449	ASN	2.1
3	P	92	VAL	2.1
3	P	275	LEU	2.1
3	P	249	SER	2.0
3	P	138	LEU	2.0
3	P	217	THR	2.0
3	P	184	PRO	2.0
3	P	69	VAL	2.0
3	P	241	VAL	2.0
3	P	435	PRO	2.0
3	P	119	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.