



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:48 AM UTC

PDB ID : 6K3F / pdb_00006k3f
Title : Crystal Structure of beta-Arrestin 2 in Complex with CXCR7 Phosphopeptide
Authors : Min, K.J.; Yoon, H.J.; Lee, H.H.
Deposited on : 2019-05-18
Resolution : 2.30 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

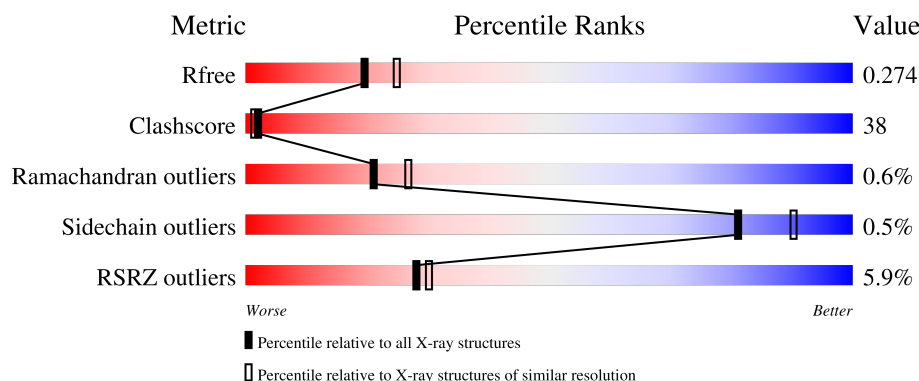
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

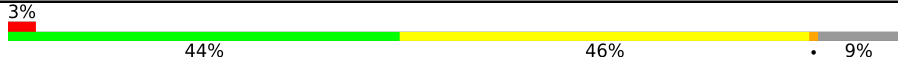
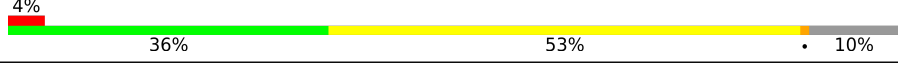
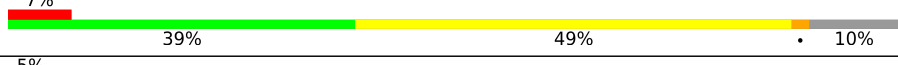
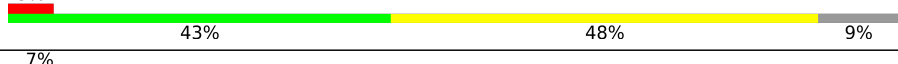
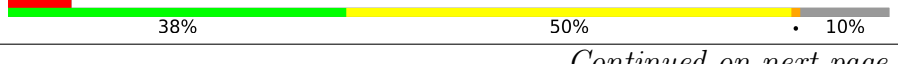
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	
1	D	377	
1	E	377	

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Mol	Chain	Length	Quality of chain
1	F	377	
2	U	15	
2	V	15	
2	W	15	
2	X	15	
2	Y	15	
2	Z	15	

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	TPO	V	338	-	-	X	-
2	TPO	Z	341	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-arrestin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2722	1733	481	497	11			
1	B	339	Total	C	N	O	S	0	0	0
			2680	1707	474	488	11			
1	C	338	Total	C	N	O	S	0	0	0
			2687	1711	476	489	11			
1	D	343	Total	C	N	O	S	0	0	0
			2722	1733	481	497	11			
1	E	339	Total	C	N	O	S	0	0	0
			2689	1711	474	493	11			
1	F	336	Total	C	N	O	S	0	0	0
			2676	1704	474	487	11			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P29067
A	-19	GLY	-	expression tag	UNP P29067
A	-18	SER	-	expression tag	UNP P29067
A	-17	SER	-	expression tag	UNP P29067
A	-16	HIS	-	expression tag	UNP P29067
A	-15	HIS	-	expression tag	UNP P29067
A	-14	HIS	-	expression tag	UNP P29067
A	-13	HIS	-	expression tag	UNP P29067
A	-12	HIS	-	expression tag	UNP P29067
A	-11	HIS	-	expression tag	UNP P29067
A	-10	SER	-	expression tag	UNP P29067
A	-9	SER	-	expression tag	UNP P29067
A	-8	GLY	-	expression tag	UNP P29067
A	-7	LEU	-	expression tag	UNP P29067
A	-6	VAL	-	expression tag	UNP P29067
A	-5	PRO	-	expression tag	UNP P29067
A	-4	ARG	-	expression tag	UNP P29067

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P29067
A	-2	SER	-	expression tag	UNP P29067
A	-1	HIS	-	expression tag	UNP P29067
A	0	MET	-	expression tag	UNP P29067
B	-20	MET	-	expression tag	UNP P29067
B	-19	GLY	-	expression tag	UNP P29067
B	-18	SER	-	expression tag	UNP P29067
B	-17	SER	-	expression tag	UNP P29067
B	-16	HIS	-	expression tag	UNP P29067
B	-15	HIS	-	expression tag	UNP P29067
B	-14	HIS	-	expression tag	UNP P29067
B	-13	HIS	-	expression tag	UNP P29067
B	-12	HIS	-	expression tag	UNP P29067
B	-11	HIS	-	expression tag	UNP P29067
B	-10	SER	-	expression tag	UNP P29067
B	-9	SER	-	expression tag	UNP P29067
B	-8	GLY	-	expression tag	UNP P29067
B	-7	LEU	-	expression tag	UNP P29067
B	-6	VAL	-	expression tag	UNP P29067
B	-5	PRO	-	expression tag	UNP P29067
B	-4	ARG	-	expression tag	UNP P29067
B	-3	GLY	-	expression tag	UNP P29067
B	-2	SER	-	expression tag	UNP P29067
B	-1	HIS	-	expression tag	UNP P29067
B	0	MET	-	expression tag	UNP P29067
C	-20	MET	-	expression tag	UNP P29067
C	-19	GLY	-	expression tag	UNP P29067
C	-18	SER	-	expression tag	UNP P29067
C	-17	SER	-	expression tag	UNP P29067
C	-16	HIS	-	expression tag	UNP P29067
C	-15	HIS	-	expression tag	UNP P29067
C	-14	HIS	-	expression tag	UNP P29067
C	-13	HIS	-	expression tag	UNP P29067
C	-12	HIS	-	expression tag	UNP P29067
C	-11	HIS	-	expression tag	UNP P29067
C	-10	SER	-	expression tag	UNP P29067
C	-9	SER	-	expression tag	UNP P29067
C	-8	GLY	-	expression tag	UNP P29067
C	-7	LEU	-	expression tag	UNP P29067
C	-6	VAL	-	expression tag	UNP P29067
C	-5	PRO	-	expression tag	UNP P29067
C	-4	ARG	-	expression tag	UNP P29067

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P29067
C	-2	SER	-	expression tag	UNP P29067
C	-1	HIS	-	expression tag	UNP P29067
C	0	MET	-	expression tag	UNP P29067
D	-20	MET	-	expression tag	UNP P29067
D	-19	GLY	-	expression tag	UNP P29067
D	-18	SER	-	expression tag	UNP P29067
D	-17	SER	-	expression tag	UNP P29067
D	-16	HIS	-	expression tag	UNP P29067
D	-15	HIS	-	expression tag	UNP P29067
D	-14	HIS	-	expression tag	UNP P29067
D	-13	HIS	-	expression tag	UNP P29067
D	-12	HIS	-	expression tag	UNP P29067
D	-11	HIS	-	expression tag	UNP P29067
D	-10	SER	-	expression tag	UNP P29067
D	-9	SER	-	expression tag	UNP P29067
D	-8	GLY	-	expression tag	UNP P29067
D	-7	LEU	-	expression tag	UNP P29067
D	-6	VAL	-	expression tag	UNP P29067
D	-5	PRO	-	expression tag	UNP P29067
D	-4	ARG	-	expression tag	UNP P29067
D	-3	GLY	-	expression tag	UNP P29067
D	-2	SER	-	expression tag	UNP P29067
D	-1	HIS	-	expression tag	UNP P29067
D	0	MET	-	expression tag	UNP P29067
E	-20	MET	-	expression tag	UNP P29067
E	-19	GLY	-	expression tag	UNP P29067
E	-18	SER	-	expression tag	UNP P29067
E	-17	SER	-	expression tag	UNP P29067
E	-16	HIS	-	expression tag	UNP P29067
E	-15	HIS	-	expression tag	UNP P29067
E	-14	HIS	-	expression tag	UNP P29067
E	-13	HIS	-	expression tag	UNP P29067
E	-12	HIS	-	expression tag	UNP P29067
E	-11	HIS	-	expression tag	UNP P29067
E	-10	SER	-	expression tag	UNP P29067
E	-9	SER	-	expression tag	UNP P29067
E	-8	GLY	-	expression tag	UNP P29067
E	-7	LEU	-	expression tag	UNP P29067
E	-6	VAL	-	expression tag	UNP P29067
E	-5	PRO	-	expression tag	UNP P29067
E	-4	ARG	-	expression tag	UNP P29067

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P29067
E	-2	SER	-	expression tag	UNP P29067
E	-1	HIS	-	expression tag	UNP P29067
E	0	MET	-	expression tag	UNP P29067
F	-20	MET	-	expression tag	UNP P29067
F	-19	GLY	-	expression tag	UNP P29067
F	-18	SER	-	expression tag	UNP P29067
F	-17	SER	-	expression tag	UNP P29067
F	-16	HIS	-	expression tag	UNP P29067
F	-15	HIS	-	expression tag	UNP P29067
F	-14	HIS	-	expression tag	UNP P29067
F	-13	HIS	-	expression tag	UNP P29067
F	-12	HIS	-	expression tag	UNP P29067
F	-11	HIS	-	expression tag	UNP P29067
F	-10	SER	-	expression tag	UNP P29067
F	-9	SER	-	expression tag	UNP P29067
F	-8	GLY	-	expression tag	UNP P29067
F	-7	LEU	-	expression tag	UNP P29067
F	-6	VAL	-	expression tag	UNP P29067
F	-5	PRO	-	expression tag	UNP P29067
F	-4	ARG	-	expression tag	UNP P29067
F	-3	GLY	-	expression tag	UNP P29067
F	-2	SER	-	expression tag	UNP P29067
F	-1	HIS	-	expression tag	UNP P29067
F	0	MET	-	expression tag	UNP P29067

- Molecule 2 is a protein called Peptide from Atypical chemokine receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	13	Total	C	N	O	P	0	0	0
			112	65	16	28	3			
2	V	12	Total	C	N	O	P	0	0	0
			104	61	15	25	3			
2	W	9	Total	C	N	O	P	0	0	0
			73	43	11	17	2			
2	X	12	Total	C	N	O	P	0	0	0
			104	61	15	25	3			
2	Y	12	Total	C	N	O	P	0	0	0
			104	61	15	25	3			
2	Z	9	Total	C	N	O	P	0	0	0
			73	43	11	17	2			

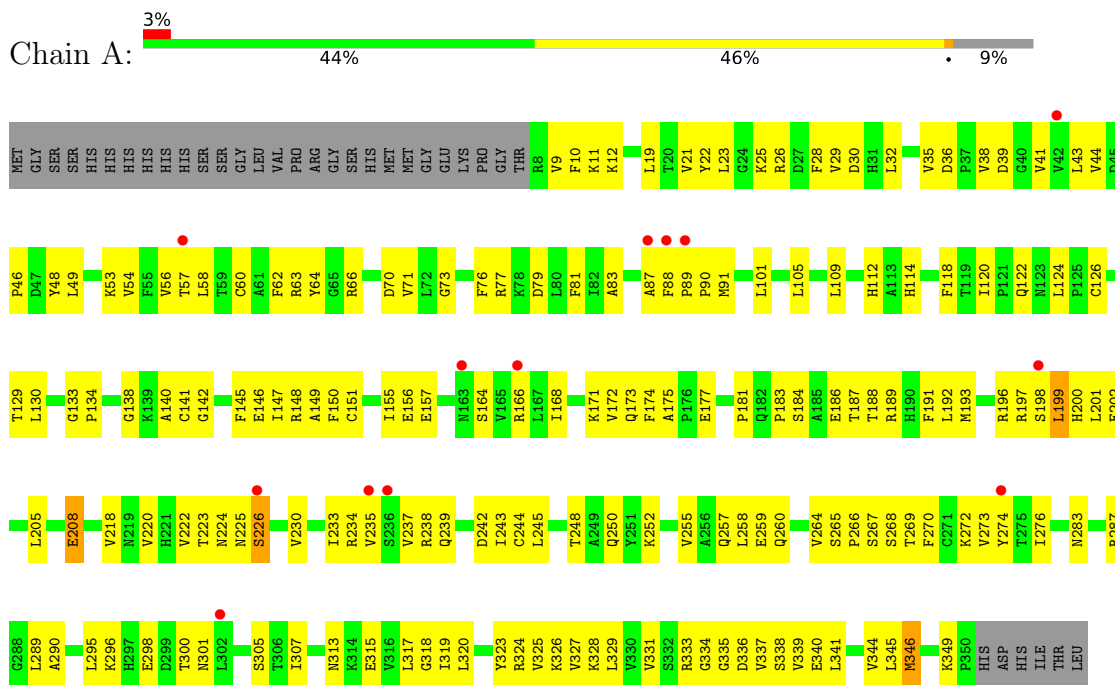
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total 85	O 85	0	0
3	U	8	Total 8	O 8	0	0
3	B	73	Total 73	O 73	0	0
3	V	6	Total 6	O 6	0	0
3	C	93	Total 93	O 93	0	0
3	W	4	Total 4	O 4	0	0
3	D	80	Total 80	O 80	0	0
3	X	2	Total 2	O 2	0	0
3	E	82	Total 82	O 82	0	0
3	Y	4	Total 4	O 4	0	0
3	F	87	Total 87	O 87	0	0

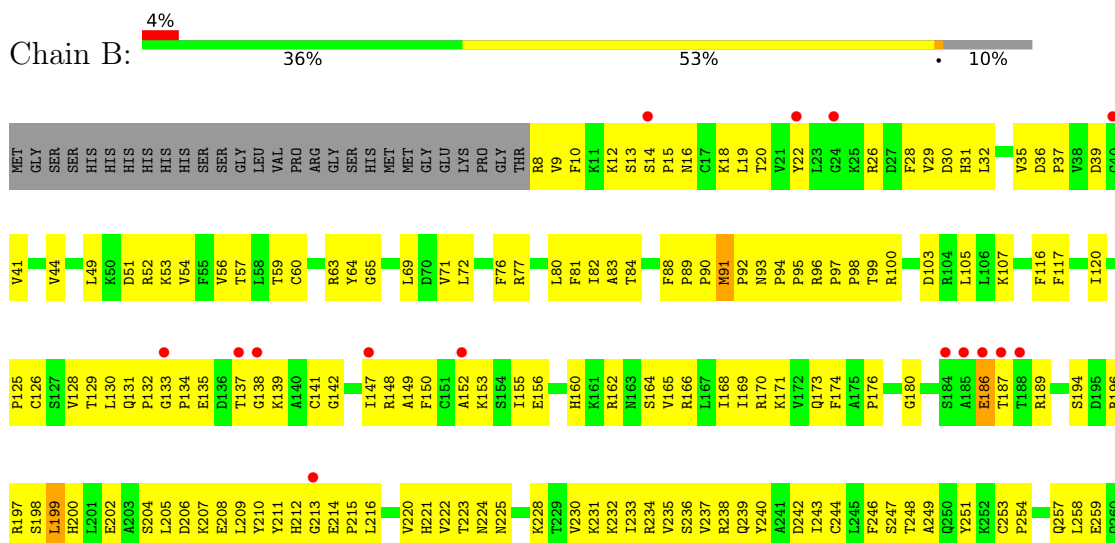
3 Residue-property plots [i](#)

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.

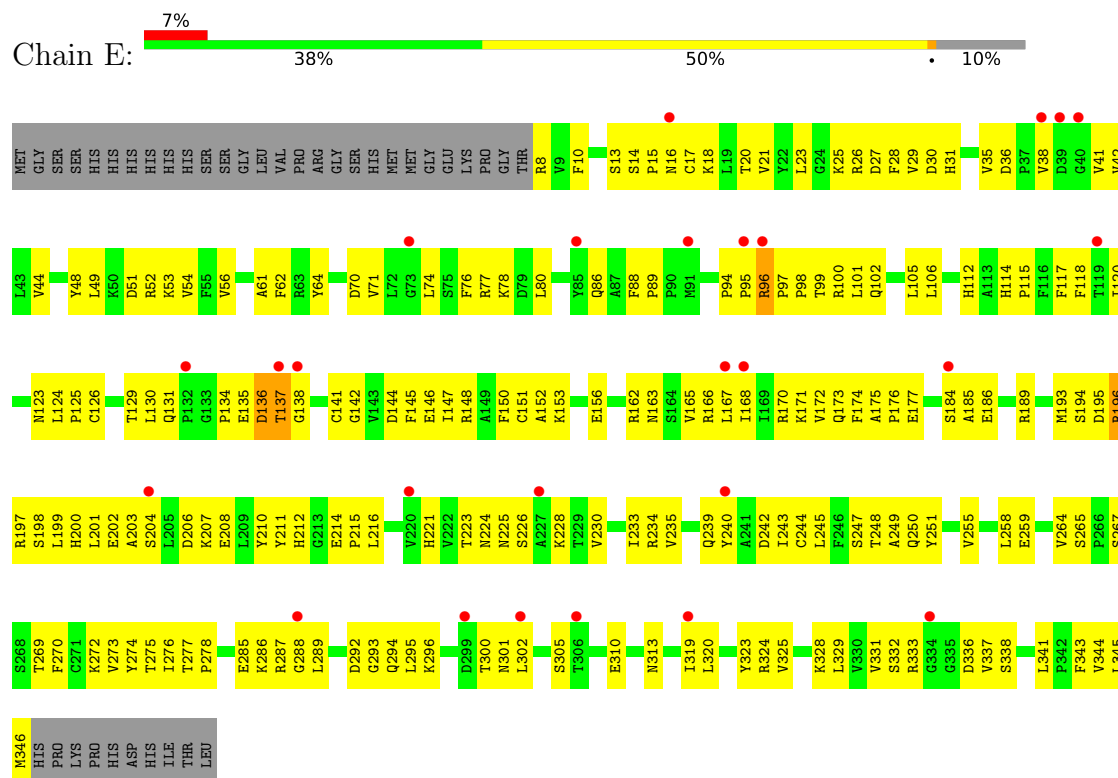
• Molecule 1: Beta-arrestin-2



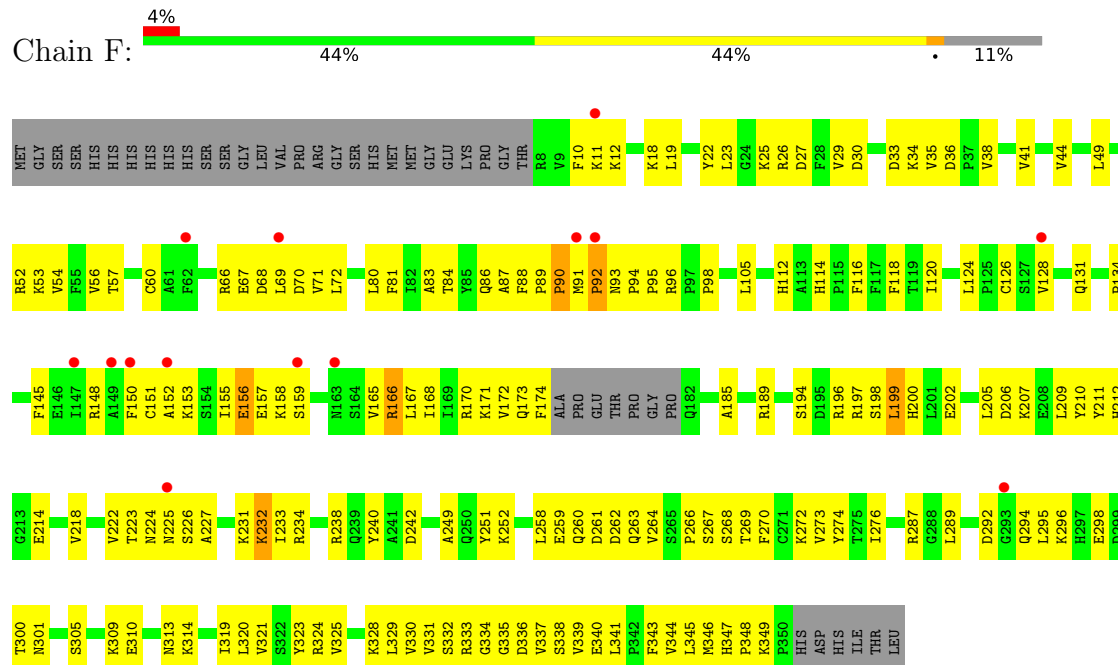
• Molecule 1: Beta-arrestin-2



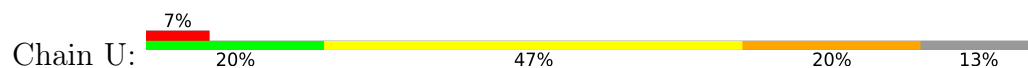
- Molecule 1: Beta-arrestin-2

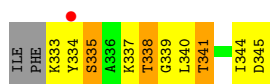


- Molecule 1: Beta-arrestin-2

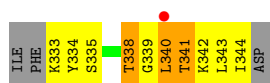
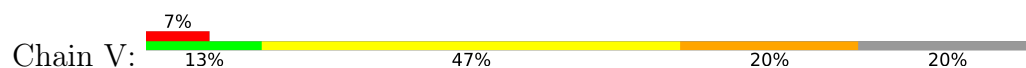


- Molecule 2: Peptide from Atypical chemokine receptor 3

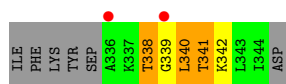




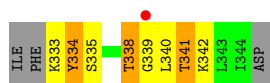
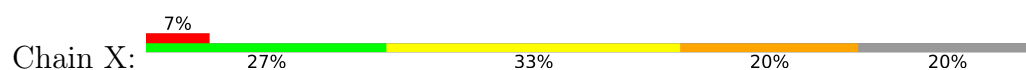
- Molecule 2: Peptide from Atypical chemokine receptor 3



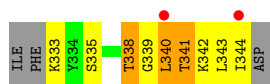
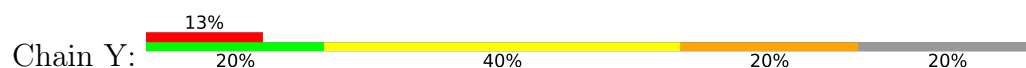
- Molecule 2: Peptide from Atypical chemokine receptor 3



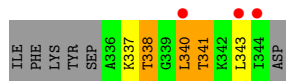
- Molecule 2: Peptide from Atypical chemokine receptor 3



- Molecule 2: Peptide from Atypical chemokine receptor 3



- Molecule 2: Peptide from Atypical chemokine receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.17Å 127.91Å 206.04Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	46.80 – 2.30 46.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.80-2.30) 99.8 (46.80-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	26.44 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.233 , 0.246 (Not available) , 0.274	Depositor DCC
R_{free} test set	5309 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17270	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: TPO, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.22	0/2784	0.65	0/3773
1	B	0.27	0/2739	0.69	1/3711 (0.0%)
1	C	0.39	3/2746 (0.1%)	0.70	1/3717 (0.0%)
1	D	0.26	0/2784	0.66	2/3773 (0.1%)
1	E	0.38	2/2748 (0.1%)	0.73	4/3723 (0.1%)
1	F	0.23	0/2734	0.62	0/3700
2	U	0.36	0/77	0.67	0/95
2	V	0.38	0/69	1.09	0/84
2	W	0.17	0/48	0.82	0/58
2	X	0.26	0/69	0.70	0/84
2	Y	0.27	0/69	0.85	0/84
2	Z	0.20	0/48	0.53	0/58
All	All	0.30	5/16915 (0.0%)	0.68	8/22860 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	6
1	D	0	1
1	E	0	1
1	F	0	4
2	U	0	1
2	W	0	1
2	X	0	1
All	All	0	20

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259	GLU	CG-CD	9.18	1.75	1.52
1	E	96	ARG	CD-NE	-8.16	1.34	1.46
1	E	96	ARG	NE-CZ	-7.37	1.25	1.33
1	C	259	GLU	CD-OE2	5.76	1.36	1.25
1	C	259	GLU	CA-CB	5.17	1.62	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	GLU	CA-CB-CG	11.05	136.20	114.10
1	E	96	ARG	NE-CZ-NH1	-10.34	111.16	121.50
1	E	96	ARG	NH1-CZ-NH2	8.62	130.50	119.30
1	E	96	ARG	CG-CD-NE	-7.69	95.09	112.00
1	D	232	LYS	CG-CD-CE	5.52	123.99	111.30
1	E	117	PHE	N-CA-C	5.25	120.17	113.18
1	B	186	GLU	N-CA-C	5.09	114.56	107.73
1	D	232	LYS	CB-CG-CD	5.05	122.92	111.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	LEU	Peptide
1	A	226	SER	Peptide
1	A	91	MET	Peptide
1	B	199	LEU	Peptide
1	B	91	MET	Peptide
1	C	199	LEU	Peptide
1	C	258	LEU	Peptide
1	C	331	VAL	Peptide
1	C	46	PRO	Peptide
1	C	92	PRO	Peptide
1	C	94	PRO	Peptide
1	D	199	LEU	Peptide
1	E	136	ASP	Peptide
1	F	166	ARG	Peptide
1	F	199	LEU	Peptide
1	F	70	ASP	Peptide
1	F	90	PRO	Peptide
2	U	337	LYS	Peptide
2	W	340	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	X	334	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2722	0	2773	240	0
1	B	2680	0	2724	259	1
1	C	2687	0	2740	232	0
1	D	2722	0	2773	226	1
1	E	2689	0	2739	244	3
1	F	2676	0	2730	213	3
2	U	112	0	105	15	0
2	V	104	0	101	23	0
2	W	73	0	76	10	0
2	X	104	0	101	7	0
2	Y	104	0	101	13	0
2	Z	73	0	77	13	0
3	A	85	0	0	3	0
3	B	73	0	0	4	0
3	C	93	0	0	8	0
3	D	80	0	0	10	0
3	E	82	0	0	7	0
3	F	87	0	0	11	1
3	U	8	0	0	0	0
3	V	6	0	0	0	0
3	W	4	0	0	1	0
3	X	2	0	0	0	0
3	Y	4	0	0	1	0
All	All	17270	0	17040	1279	5

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 38.

All (1279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLU:CD	1:C:259:GLU:CG	1.75	1.57
1:A:337:VAL:HB	1:B:135:GLU:OE2	1.21	1.31
1:A:233:ILE:HD13	1:A:329:LEU:CG	1.76	1.14
1:F:91:MET:HG3	1:F:92:PRO:HD3	1.25	1.14
1:C:238:ARG:HE	1:C:326:LYS:HD3	1.08	1.12
1:A:233:ILE:CD1	1:A:329:LEU:HG	1.83	1.08
1:C:53:LYS:HD2	1:C:89:PRO:HD3	1.39	1.04
1:F:212:HIS:CE1	1:F:301:ASN:HB2	1.94	1.03
1:F:12:LYS:NZ	2:Z:341:TPO:O3P	1.91	1.02
1:D:168:ILE:HD11	1:D:296:LYS:HE2	1.42	1.01
1:F:12:LYS:CD	2:Z:341:TPO:O3P	2.09	1.01
1:B:180:GLY:N	1:B:208:GLU:OE2	1.93	1.01
1:C:234:ARG:NH2	1:C:259:GLU:OE2	1.93	1.00
1:B:53:LYS:HD2	1:B:89:PRO:HD3	1.43	1.00
1:C:297:HIS:HB3	2:W:342:LYS:HE3	1.46	0.96
1:E:168:ILE:HD11	1:E:296:LYS:HZ3	1.30	0.96
1:D:232:LYS:HA	1:D:232:LYS:HE2	1.50	0.94
1:A:270:PHE:HA	1:C:349:LYS:HB3	1.51	0.93
1:C:238:ARG:NE	1:C:326:LYS:HD3	1.81	0.93
1:D:200:HIS:HB2	1:D:223:THR:HB	1.50	0.93
1:F:92:PRO:HG2	1:F:94:PRO:HB3	1.51	0.92
1:C:238:ARG:HE	1:C:326:LYS:CD	1.82	0.91
1:C:258:LEU:CD1	1:C:276:ILE:HA	2.00	0.91
1:B:232:LYS:NZ	1:B:261:ASP:HA	1.85	0.91
1:E:53:LYS:HD2	1:E:89:PRO:HD3	1.52	0.91
1:F:12:LYS:HD3	2:Z:341:TPO:O3P	1.71	0.91
1:F:90:PRO:O	1:F:93:ASN:N	2.04	0.90
1:E:151:CYS:O	1:E:163:ASN:ND2	2.05	0.90
1:B:211:TYR:HB2	1:E:211:TYR:HB2	1.55	0.89
1:F:300:THR:HG22	1:F:301:ASN:H	1.38	0.89
1:E:244:CYS:HG	1:E:248:THR:HG1	1.07	0.88
1:F:328:LYS:HE3	1:F:336:ASP:HB3	1.56	0.87
1:B:148:ARG:HA	1:B:165:VAL:O	1.74	0.87
1:C:48:TYR:O	1:C:52:ARG:NH1	2.07	0.87
1:B:166:ARG:NH2	2:V:339:GLY:H	1.73	0.86
1:A:233:ILE:HD13	1:A:329:LEU:HG	0.89	0.86
2:V:343:LEU:HD22	1:D:192:LEU:CD1	2.06	0.86
1:A:200:HIS:HB2	1:A:223:THR:HB	1.57	0.86
1:E:196:ARG:HD2	1:E:226:SER:HA	1.58	0.85
1:F:86:GLN:HG3	1:F:91:MET:HE3	1.59	0.85
1:A:337:VAL:CB	1:B:135:GLU:OE2	2.17	0.85
1:D:329:LEU:HD22	1:E:135:GLU:HG3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HH12	2:U:338:TPO:P	1.99	0.84
1:F:12:LYS:HD3	2:Z:341:TPO:P	2.17	0.84
1:D:328:LYS:HE3	1:D:336:ASP:HB3	1.57	0.84
1:F:258:LEU:HD12	1:F:276:ILE:HA	1.56	0.84
1:B:200:HIS:HB2	1:B:223:THR:HB	1.59	0.84
1:B:166:ARG:HE	2:V:338:TPO:HB	1.39	0.83
1:C:29:VAL:HG13	1:C:174:PHE:HB2	1.60	0.83
1:D:266:PRO:HD2	1:F:33:ASP:HB2	1.59	0.82
1:C:231:LYS:O	1:C:232:LYS:HB2	1.78	0.82
1:F:225:ASN:O	1:F:267:SER:N	2.11	0.81
2:V:343:LEU:HD22	1:D:192:LEU:HD13	1.62	0.81
1:D:151:CYS:O	1:D:163:ASN:ND2	2.12	0.81
1:F:53:LYS:HG3	1:F:89:PRO:HD3	1.63	0.81
1:D:26:ARG:HD2	1:D:295:LEU:HD13	1.63	0.80
1:A:242:ASP:CG	1:B:247:SER:HB3	2.06	0.80
1:A:250:GLN:N	1:B:248:THR:O	2.14	0.80
1:A:250:GLN:HB2	1:B:249:ALA:HA	1.63	0.80
1:F:91:MET:HG3	1:F:92:PRO:CD	2.08	0.80
1:A:148:ARG:HH21	1:A:166:ARG:HG2	1.45	0.80
1:D:250:GLN:N	1:E:248:THR:O	2.13	0.79
1:D:337:VAL:HA	1:E:287:ARG:HD2	1.64	0.79
1:F:231:LYS:HB3	1:F:330:VAL:HG23	1.64	0.79
1:B:15:PRO:HA	1:C:223:THR:HG23	1.65	0.78
1:E:38:VAL:HB	1:E:118:PHE:HB2	1.65	0.78
1:F:222:VAL:HG11	1:F:264:VAL:HG21	1.65	0.78
2:V:343:LEU:HD21	1:D:192:LEU:HD12	1.64	0.78
1:D:175:ALA:O	1:D:349:LYS:NZ	2.17	0.78
1:F:272:LYS:NZ	1:F:273:VAL:O	2.15	0.78
1:A:328:LYS:HE2	1:A:336:ASP:HB3	1.66	0.78
1:C:258:LEU:HD12	1:C:276:ILE:HA	1.66	0.78
1:B:196:ARG:NH1	1:B:225:ASN:O	2.18	0.77
1:C:186:GLU:HB2	1:C:202:GLU:HG3	1.66	0.77
1:D:29:VAL:HG11	1:D:350:PRO:HD2	1.65	0.77
1:E:168:ILE:HD11	1:E:296:LYS:NZ	2.00	0.77
2:V:343:LEU:CD2	1:D:192:LEU:HD12	2.15	0.77
1:D:197:ARG:HG2	1:D:225:ASN:HD21	1.49	0.77
1:F:12:LYS:CE	2:Z:341:TPO:O3P	2.33	0.77
1:B:59:THR:HA	1:B:82:ILE:HD12	1.64	0.76
1:C:35:VAL:HG11	1:C:120:ILE:HB	1.67	0.76
1:E:185:ALA:HB3	1:E:203:ALA:HB3	1.66	0.75
1:F:168:ILE:HD13	1:F:296:LYS:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ARG:HA	1:D:103:ASP:HB2	1.68	0.75
1:C:295:LEU:HB3	1:C:296:LYS:HZ2	1.51	0.75
1:A:58:LEU:HG	1:A:147:ILE:HG22	1.69	0.75
1:C:272:LYS:NZ	1:C:273:VAL:O	2.19	0.75
1:D:196:ARG:HH21	1:D:227:ALA:H	1.33	0.75
1:D:96:ARG:NH1	3:D:401:HOH:O	2.19	0.74
1:D:174:PHE:HB2	1:D:349:LYS:HG2	1.67	0.74
1:F:38:VAL:HB	1:F:118:PHE:HB2	1.70	0.74
1:B:35:VAL:HG11	1:B:120:ILE:HB	1.68	0.74
1:D:208:GLU:HG3	1:D:209:LEU:HD12	1.69	0.74
2:Z:338:TPO:HG22	2:Z:340:LEU:HD13	1.70	0.74
1:A:268:SER:HB2	1:C:32:LEU:HD11	1.69	0.74
1:F:134:PRO:HD3	1:F:287:ARG:HB2	1.69	0.74
1:F:12:LYS:HE2	1:F:166:ARG:O	1.87	0.74
1:D:185:ALA:HB1	1:E:137:THR:HG23	1.69	0.74
1:B:64:TYR:H	1:B:77:ARG:HH11	1.36	0.74
1:C:174:PHE:HA	1:C:347:HIS:HB2	1.69	0.74
1:A:338:SER:HB3	1:B:287:ARG:CZ	2.19	0.73
2:V:343:LEU:CD2	1:D:192:LEU:CD1	2.65	0.73
1:C:200:HIS:HB2	1:C:223:THR:HB	1.68	0.73
1:C:296:LYS:HB3	2:W:340:LEU:HD22	1.70	0.73
1:D:284:ARG:HG2	1:D:285:GLU:HG3	1.70	0.73
1:C:192:LEU:HD13	1:F:313:ASN:HD21	1.54	0.73
1:F:12:LYS:HD3	2:Z:341:TPO:O1P	1.88	0.73
1:D:232:LYS:HD2	1:D:261:ASP:HA	1.70	0.73
1:F:232:LYS:HD3	1:F:261:ASP:HA	1.69	0.73
1:B:166:ARG:HH21	2:V:338:TPO:HG23	1.53	0.73
1:C:66:ARG:HB2	1:C:69:LEU:HB3	1.70	0.73
1:C:193:MET:O	1:C:228:LYS:NZ	2.21	0.73
1:F:44:VAL:O	1:F:112:HIS:ND1	2.22	0.73
1:E:18:LYS:O	1:E:44:VAL:HA	1.89	0.73
1:A:130:LEU:HD11	1:A:243:ILE:HG12	1.71	0.73
1:C:238:ARG:HH11	1:C:238:ARG:HG2	1.52	0.73
1:D:233:ILE:HG13	1:D:329:LEU:HG	1.71	0.73
1:F:166:ARG:NH2	3:F:402:HOH:O	2.22	0.72
1:C:333:ARG:O	1:C:333:ARG:NE	2.22	0.72
1:A:233:ILE:HD12	1:A:328:LYS:O	1.89	0.72
1:C:232:LYS:HE2	1:C:262:ASP:H	1.55	0.72
1:C:196:ARG:NH1	1:C:226:SER:O	2.23	0.72
1:A:130:LEU:HD23	1:A:141:CYS:HB3	1.72	0.72
1:C:54:VAL:HB	1:C:88:PHE:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:SER:HA	1:B:20:THR:HG23	1.70	0.72
1:E:14:SER:HB2	1:E:165:VAL:HG22	1.71	0.72
1:F:12:LYS:CD	2:Z:341:TPO:P	2.78	0.71
1:C:234:ARG:NH1	1:C:257:GLN:HG3	2.06	0.71
1:F:238:ARG:NH1	3:F:401:HOH:O	2.19	0.71
1:B:225:ASN:HA	1:B:267:SER:H	1.55	0.71
1:F:44:VAL:HG21	1:F:49:LEU:HD13	1.71	0.71
1:A:269:THR:HG21	1:C:211:TYR:CZ	2.26	0.71
1:E:272:LYS:NZ	1:E:273:VAL:O	2.22	0.70
1:B:166:ARG:NH2	2:V:339:GLY:N	2.38	0.70
1:C:187:THR:O	1:C:200:HIS:HA	1.91	0.70
1:C:259:GLU:CD	1:C:259:GLU:CB	2.63	0.70
1:A:23:LEU:HD21	1:A:147:ILE:HD11	1.74	0.70
1:F:86:GLN:HG3	1:F:91:MET:CE	2.22	0.70
1:A:79:ASP:OD1	3:A:401:HOH:O	2.08	0.70
1:A:328:LYS:HA	1:A:338:SER:HB2	1.74	0.70
1:C:70:ASP:HB3	1:C:77:ARG:HH22	1.56	0.70
1:E:126:CYS:SG	1:E:173:GLN:N	2.64	0.70
1:E:234:ARG:NH1	3:E:404:HOH:O	2.22	0.69
1:A:233:ILE:HG23	1:A:274:TYR:CE2	2.26	0.69
1:B:205:LEU:HD11	1:B:324:ARG:HH22	1.57	0.69
1:E:225:ASN:O	1:E:225:ASN:ND2	2.25	0.69
1:C:264:VAL:HG13	1:C:270:PHE:HB2	1.73	0.69
1:E:96:ARG:HG3	1:E:97:PRO:HD3	1.75	0.69
1:C:239:GLN:HE22	1:C:290:ALA:HB3	1.57	0.69
1:E:234:ARG:HB3	1:E:328:LYS:HD2	1.72	0.69
1:D:225:ASN:HA	1:D:267:SER:HA	1.74	0.69
1:A:148:ARG:NH2	1:A:166:ARG:HG2	2.08	0.68
1:C:91:MET:O	1:C:93:ASN:N	2.27	0.68
1:F:49:LEU:HG	1:F:52:ARG:HB3	1.76	0.68
1:A:338:SER:H	1:B:287:ARG:HD2	1.59	0.68
1:B:341:LEU:HD12	1:B:342:PRO:HD2	1.75	0.68
1:D:131:GLN:NE2	1:D:286:LYS:O	2.27	0.68
1:B:230:VAL:HG23	1:B:231:LYS:H	1.59	0.68
1:B:18:LYS:O	1:B:44:VAL:HA	1.94	0.68
1:D:175:ALA:N	1:D:347:HIS:O	2.26	0.68
1:B:96:ARG:O	1:B:98:PRO:HD3	1.93	0.68
1:F:194:SER:OG	1:F:196:ARG:NH2	2.27	0.68
1:C:292:ASP:OD2	1:C:301:ASN:ND2	2.27	0.68
1:E:324:ARG:HD2	1:E:341:LEU:O	1.93	0.68
1:B:162:ARG:O	1:C:269:THR:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:O	1:C:332:SER:N	2.28	0.67
2:Y:339:GLY:O	2:Y:340:LEU:HB2	1.94	0.67
1:C:104:ARG:NH1	3:C:404:HOH:O	2.27	0.67
1:A:296:LYS:HD3	2:U:341:TPO:P	2.35	0.67
1:A:198:SER:O	1:A:199:LEU:HG	1.93	0.67
1:B:234:ARG:HA	1:B:259:GLU:HB3	1.77	0.67
1:B:149:ALA:O	1:B:164:SER:HA	1.94	0.67
1:D:96:ARG:HB3	1:D:97:PRO:HD3	1.76	0.67
1:E:16:ASN:HD21	1:E:18:LYS:HB3	1.59	0.67
1:E:210:TYR:CD1	1:E:214:GLU:HG3	2.30	0.67
1:D:44:VAL:HG11	1:D:54:VAL:HG21	1.75	0.67
1:E:196:ARG:O	1:E:198:SER:OG	2.06	0.67
1:D:53:LYS:HG3	1:D:89:PRO:HD3	1.76	0.67
1:B:16:ASN:ND2	1:C:269:THR:OG1	2.24	0.66
1:F:172:VAL:HG23	1:F:174:PHE:HE1	1.59	0.66
1:B:272:LYS:NZ	1:B:273:VAL:O	2.27	0.66
1:A:196:ARG:HD3	1:A:226:SER:HB3	1.77	0.66
1:B:194:SER:OG	1:B:196:ARG:NH2	2.28	0.66
1:D:194:SER:HB3	1:D:196:ARG:HH12	1.61	0.66
1:E:44:VAL:HG11	1:E:54:VAL:HG21	1.77	0.66
1:A:337:VAL:HB	1:B:135:GLU:CD	2.14	0.66
1:B:162:ARG:HA	1:C:269:THR:O	1.95	0.66
1:E:25:LYS:NZ	1:E:36:ASP:OD2	2.28	0.66
1:B:16:ASN:OD1	1:B:18:LYS:HB2	1.96	0.66
1:E:305:SER:N	1:E:345:LEU:O	2.29	0.66
1:D:174:PHE:CD2	1:D:347:HIS:HB3	2.31	0.66
1:E:200:HIS:HB2	1:E:223:THR:HB	1.76	0.66
1:F:131:GLN:HB2	1:F:289:LEU:O	1.96	0.66
1:A:238:ARG:N	1:A:324:ARG:O	2.20	0.66
1:B:324:ARG:HD3	1:B:341:LEU:C	2.21	0.66
1:E:175:ALA:HB2	1:E:346:MET:HB2	1.76	0.66
1:C:148:ARG:NH1	3:C:406:HOH:O	2.28	0.65
1:C:258:LEU:HD13	1:C:275:THR:O	1.96	0.65
1:B:100:ARG:HA	1:B:103:ASP:HB2	1.78	0.65
1:E:235:VAL:HG21	1:E:274:TYR:HB3	1.78	0.65
1:A:175:ALA:HB2	1:A:346:MET:HB3	1.77	0.65
1:A:189:ARG:NH2	1:A:196:ARG:O	2.29	0.65
1:B:242:ASP:HB3	1:B:320:LEU:O	1.95	0.65
1:E:35:VAL:HG11	1:E:120:ILE:HB	1.78	0.65
1:A:148:ARG:NH1	2:U:335:SEP:O2P	2.30	0.65
1:B:166:ARG:HH21	2:V:338:TPO:CG2	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:VAL:HG21	1:E:135:GLU:H	1.59	0.65
1:B:32:LEU:HD11	1:B:176:PRO:HA	1.78	0.65
1:A:189:ARG:O	1:A:189:ARG:NH1	2.28	0.65
1:A:199:LEU:HD22	1:B:135:GLU:CG	2.25	0.65
1:B:236:SER:HA	1:B:257:GLN:HB3	1.77	0.65
1:C:160:HIS:O	1:C:164:SER:OG	2.11	0.65
1:D:339:VAL:HG11	1:E:137:THR:HB	1.78	0.65
1:E:120:ILE:HG21	1:E:171:LYS:HE3	1.79	0.65
1:C:41:VAL:HG22	1:C:105:LEU:HD13	1.78	0.65
1:E:16:ASN:OD1	1:F:267:SER:C	2.39	0.65
1:A:38:VAL:HB	1:A:118:PHE:HB2	1.78	0.65
1:D:38:VAL:HB	1:D:118:PHE:HB2	1.79	0.65
1:A:337:VAL:HG13	1:B:287:ARG:HB2	1.78	0.65
1:D:114:HIS:N	3:D:405:HOH:O	2.30	0.65
1:F:240:TYR:OH	1:F:340:GLU:OE2	2.14	0.65
1:A:64:TYR:CD2	1:A:245:LEU:HD11	2.32	0.64
1:B:76:PHE:HB2	2:V:333:LYS:N	2.12	0.64
1:B:242:ASP:O	1:B:320:LEU:N	2.30	0.64
1:A:242:ASP:HB3	1:A:320:LEU:H	1.63	0.64
1:E:185:ALA:O	1:E:203:ALA:N	2.29	0.64
1:F:67:GLU:O	1:F:71:VAL:HB	1.98	0.64
1:A:235:VAL:HG21	1:A:274:TYR:HB3	1.80	0.64
1:E:162:ARG:HA	1:F:269:THR:H	1.63	0.64
1:F:212:HIS:NE2	1:F:301:ASN:HB2	2.12	0.64
1:F:168:ILE:HG22	1:F:295:LEU:HD23	1.79	0.64
1:A:252:LYS:HD3	1:B:251:TYR:CD1	2.33	0.64
2:Y:333:LYS:N	3:Y:401:HOH:O	2.31	0.64
1:F:60:CYS:HB3	1:F:81:PHE:HB3	1.80	0.64
1:A:326:LYS:HD2	1:B:287:ARG:HH22	1.62	0.64
1:A:295:LEU:HB3	1:A:296:LYS:HZ1	1.61	0.64
1:C:310:GLU:CD	1:C:310:GLU:H	2.05	0.64
1:D:72:LEU:HD12	1:D:72:LEU:O	1.96	0.64
1:E:15:PRO:HG3	1:F:223:THR:CG2	2.28	0.64
1:A:295:LEU:HB2	1:A:298:GLU:HG2	1.80	0.63
1:C:226:SER:C	1:C:228:LYS:H	2.04	0.63
1:C:234:ARG:HH21	1:C:259:GLU:CD	2.06	0.63
1:B:243:ILE:HG12	1:B:319:ILE:HG12	1.80	0.63
1:D:287:ARG:NH2	3:D:404:HOH:O	2.30	0.63
2:V:343:LEU:HD23	1:D:193:MET:HB2	1.81	0.63
1:E:186:GLU:HA	1:E:201:LEU:O	1.99	0.63
1:A:126:CYS:SG	1:A:173:GLN:HB2	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:HB	1:B:88:PHE:HB3	1.80	0.63
1:B:170:ARG:NH1	1:B:293:GLY:O	2.32	0.63
1:A:71:VAL:HG21	2:U:334:TYR:CZ	2.34	0.63
1:E:131:GLN:HB3	1:E:289:LEU:H	1.62	0.63
1:F:57:THR:HG1	1:F:150:PHE:HE2	1.46	0.63
1:D:63:ARG:NH2	1:D:141:CYS:O	2.31	0.63
1:B:14:SER:HB3	1:B:19:LEU:O	1.98	0.63
1:C:12:LYS:HE3	2:W:341:TPO:HG22	1.81	0.63
1:D:174:PHE:CB	1:D:349:LYS:HG2	2.28	0.63
1:D:194:SER:HB2	1:D:228:LYS:HE2	1.81	0.63
1:E:224:ASN:ND2	1:E:265:SER:O	2.32	0.63
1:F:324:ARG:NE	1:F:325:VAL:H	1.96	0.63
1:E:162:ARG:NH2	3:E:409:HOH:O	2.32	0.62
1:E:148:ARG:NE	1:E:166:ARG:HB3	2.14	0.62
1:F:252:LYS:HD3	1:F:252:LYS:H	1.63	0.62
1:A:181:PRO:HB3	1:B:72:LEU:HD12	1.81	0.62
1:A:295:LEU:HB3	1:A:296:LYS:NZ	2.15	0.62
1:F:305:SER:HA	1:F:321:VAL:HG12	1.81	0.62
1:A:269:THR:HG21	1:C:211:TYR:CE2	2.35	0.62
1:B:234:ARG:HH12	1:E:100:ARG:NH2	1.96	0.62
1:F:131:GLN:HB3	1:F:289:LEU:H	1.64	0.62
1:A:338:SER:OG	1:A:339:VAL:N	2.32	0.62
1:E:15:PRO:HB3	1:F:223:THR:HG22	1.82	0.62
1:E:197:ARG:NH2	3:E:407:HOH:O	2.29	0.62
1:D:49:LEU:HG	1:D:52:ARG:HB3	1.82	0.62
1:D:146:GLU:CG	1:D:168:ILE:HG22	2.30	0.62
1:C:88:PHE:HD2	1:C:114:HIS:CE1	2.17	0.62
1:C:131:GLN:HB3	1:C:289:LEU:H	1.64	0.62
1:D:234:ARG:HH11	1:D:234:ARG:HG3	1.65	0.62
1:A:9:VAL:HG21	1:A:105:LEU:HD21	1.82	0.61
1:A:76:PHE:CG	1:A:77:ARG:N	2.67	0.61
1:A:248:THR:C	1:B:248:THR:HB	2.25	0.61
1:B:196:ARG:HD2	1:B:225:ASN:O	2.00	0.61
1:C:239:GLN:NE2	1:C:290:ALA:HB3	2.15	0.61
1:E:185:ALA:O	1:E:202:GLU:HA	1.99	0.61
1:C:200:HIS:HB2	1:C:223:THR:CB	2.30	0.61
1:A:224:ASN:ND2	1:A:265:SER:O	2.33	0.61
1:D:146:GLU:HG2	1:D:168:ILE:HA	1.82	0.61
1:D:168:ILE:CD1	1:D:296:LYS:HE2	2.25	0.61
1:D:250:GLN:OE1	1:E:249:ALA:HB2	2.00	0.61
1:F:148:ARG:HD2	1:F:166:ARG:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:HIS:O	1:F:223:THR:HB	1.99	0.61
1:B:59:THR:HB	1:B:82:ILE:CD1	2.31	0.61
1:B:207:LYS:HB2	1:B:210:TYR:CE1	2.36	0.61
1:D:120:ILE:HG23	1:D:124:LEU:HD22	1.82	0.61
1:D:196:ARG:HH21	1:D:227:ALA:N	1.97	0.61
1:D:196:ARG:NH2	1:D:227:ALA:H	1.99	0.61
1:D:210:TYR:CD1	1:D:214:GLU:HG3	2.35	0.61
1:E:16:ASN:ND2	1:E:18:LYS:HB3	2.15	0.61
1:A:337:VAL:HG11	1:B:134:PRO:N	2.15	0.61
1:C:150:PHE:HB2	1:C:163:ASN:HD22	1.66	0.61
1:D:170:ARG:NH1	1:D:293:GLY:O	2.32	0.61
1:D:255:VAL:O	1:D:283:ASN:ND2	2.25	0.61
1:F:330:VAL:HA	1:F:335:GLY:O	2.01	0.61
1:B:59:THR:CA	1:B:82:ILE:HD12	2.30	0.61
1:B:224:ASN:ND2	1:B:265:SER:O	2.34	0.61
1:C:295:LEU:HB3	1:C:296:LYS:NZ	2.15	0.61
1:D:201:LEU:HD21	1:D:220:VAL:HG23	1.83	0.61
1:E:130:LEU:HD22	1:E:319:ILE:CD1	2.29	0.61
1:F:324:ARG:HD3	1:F:341:LEU:C	2.26	0.61
1:B:206:ASP:HB2	1:E:177:GLU:CB	2.30	0.61
1:D:187:THR:HB	1:E:138:GLY:HA2	1.83	0.61
1:E:292:ASP:OD2	1:E:301:ASN:ND2	2.33	0.61
1:C:296:LYS:HE2	2:W:342:LYS:HA	1.82	0.61
1:B:230:VAL:O	1:B:331:VAL:HA	2.00	0.61
1:D:250:GLN:NE2	1:E:247:SER:HB3	2.16	0.61
1:B:166:ARG:HH21	2:V:338:TPO:CB	2.14	0.60
1:E:131:GLN:NE2	1:E:286:LYS:O	2.34	0.60
1:E:170:ARG:HB2	1:E:295:LEU:HD21	1.83	0.60
1:F:305:SER:N	1:F:345:LEU:O	2.33	0.60
1:B:15:PRO:CA	1:C:223:THR:HG23	2.30	0.60
1:C:126:CYS:SG	1:C:173:GLN:HG3	2.41	0.60
1:D:186:GLU:OE2	1:D:200:HIS:ND1	2.34	0.60
1:E:305:SER:O	1:E:346:MET:HG2	2.01	0.60
1:D:146:GLU:CD	1:D:168:ILE:HG22	2.26	0.60
1:B:148:ARG:NE	1:B:166:ARG:HB3	2.16	0.60
1:E:30:ASP:HB3	1:E:172:VAL:O	2.02	0.60
1:E:150:PHE:HB2	1:E:163:ASN:OD1	2.02	0.60
1:F:34:LYS:NZ	3:F:406:HOH:O	2.31	0.60
1:F:35:VAL:HG11	1:F:120:ILE:HB	1.83	0.60
1:B:275:THR:HB	1:E:31:HIS:CE1	2.37	0.60
1:D:232:LYS:HA	1:D:232:LYS:CE	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLY:HA2	1:E:8:ARG:HH22	1.67	0.60
1:B:197:ARG:NH1	3:B:405:HOH:O	2.33	0.60
1:D:339:VAL:CG1	1:E:137:THR:HB	2.31	0.60
1:F:226:SER:O	1:F:266:PRO:HB3	2.02	0.60
1:A:200:HIS:HE2	1:C:180:GLY:N	1.99	0.60
1:B:76:PHE:O	1:B:77:ARG:NE	2.35	0.60
1:B:18:LYS:HB3	1:B:19:LEU:HD12	1.83	0.60
1:A:324:ARG:HD3	1:A:341:LEU:C	2.27	0.59
2:V:338:TPO:HA	1:C:221:HIS:CD2	2.37	0.59
1:A:233:ILE:HD13	1:A:329:LEU:CD1	2.32	0.59
1:D:131:GLN:HB3	1:D:289:LEU:H	1.68	0.59
1:F:210:TYR:HD2	1:F:214:GLU:HB2	1.66	0.59
1:B:80:LEU:HD21	1:B:125:PRO:HD2	1.84	0.59
1:B:244:CYS:N	1:B:318:GLY:O	2.34	0.59
1:F:90:PRO:HG3	1:F:114:HIS:HE1	1.67	0.59
1:E:44:VAL:HG23	1:E:112:HIS:ND1	2.17	0.59
1:E:112:HIS:O	1:E:114:HIS:ND1	2.34	0.59
2:V:339:GLY:O	2:V:340:LEU:HB2	2.02	0.59
1:C:185:ALA:O	1:C:202:GLU:HA	2.03	0.59
1:D:52:ARG:NH2	1:D:152:ALA:O	2.36	0.59
1:E:230:VAL:HG13	1:E:331:VAL:HG22	1.85	0.59
1:A:296:LYS:HD3	2:U:341:TPO:O1P	2.02	0.59
1:B:202:GLU:CD	1:B:204:SER:HB2	2.28	0.59
1:E:328:LYS:HA	1:E:338:SER:HB2	1.84	0.59
1:E:329:LEU:O	1:E:336:ASP:HA	2.01	0.59
1:A:226:SER:O	1:A:266:PRO:HB3	2.02	0.59
1:F:29:VAL:HG13	1:F:174:PHE:CG	2.38	0.59
1:D:35:VAL:HG11	1:D:120:ILE:HB	1.85	0.58
1:F:52:ARG:NH2	1:F:152:ALA:O	2.36	0.58
1:C:44:VAL:HG12	1:C:112:HIS:NE2	2.17	0.58
1:A:199:LEU:HD22	1:B:135:GLU:HG2	1.84	0.58
1:A:250:GLN:NE2	1:B:247:SER:OG	2.28	0.58
1:B:208:GLU:CD	1:B:209:LEU:HD12	2.29	0.58
1:F:44:VAL:HG13	1:F:112:HIS:CE1	2.38	0.58
1:E:294:GLN:HB3	1:E:300:THR:HB	1.84	0.58
1:F:172:VAL:HG23	1:F:174:PHE:CE1	2.38	0.58
1:D:154:SER:OG	1:D:158:LYS:HB3	2.03	0.58
1:A:11:LYS:HA	1:A:21:VAL:O	2.04	0.58
1:A:186:GLU:HA	1:A:201:LEU:O	2.03	0.58
2:U:333:LYS:HG3	2:U:334:TYR:HD1	1.69	0.58
1:B:26:ARG:HH12	2:V:343:LEU:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLY:HA2	1:B:139:LYS:HD2	1.85	0.58
1:B:96:ARG:HB2	1:B:97:PRO:HD3	1.86	0.58
1:C:204:SER:HB3	1:C:221:HIS:HE1	1.69	0.58
1:B:242:ASP:OD1	1:B:248:THR:HG23	2.03	0.58
1:C:259:GLU:CG	1:C:259:GLU:OE1	2.44	0.58
1:D:189:ARG:HG2	1:E:136:ASP:OD2	2.03	0.58
1:D:239:GLN:HG3	1:D:323:TYR:CE2	2.39	0.58
1:F:10:PHE:CE1	1:F:23:LEU:HB2	2.39	0.58
1:D:339:VAL:HG21	1:E:137:THR:H	1.68	0.57
1:C:297:HIS:ND1	3:C:411:HOH:O	2.32	0.57
1:F:12:LYS:HZ1	1:F:166:ARG:C	2.12	0.57
1:A:268:SER:CB	1:C:32:LEU:HD11	2.34	0.57
1:C:232:LYS:HD3	1:C:263:GLN:H	1.68	0.57
1:D:201:LEU:HB3	1:E:136:ASP:O	2.04	0.57
1:E:186:GLU:HB2	1:E:202:GLU:HG3	1.84	0.57
1:D:328:LYS:HA	1:D:338:SER:HB2	1.86	0.57
1:F:211:TYR:HB3	1:F:346:MET:O	2.05	0.57
1:B:29:VAL:HB	1:B:31:HIS:CE1	2.40	0.57
1:B:202:GLU:O	1:B:220:VAL:HA	2.05	0.57
1:D:272:LYS:NZ	1:D:273:VAL:O	2.28	0.57
1:A:269:THR:HG21	1:C:211:TYR:OH	2.04	0.57
1:B:116:PHE:CE1	1:B:147:ILE:HD11	2.40	0.57
1:B:197:ARG:HD2	1:B:200:HIS:NE2	2.20	0.57
1:E:13:SER:HA	1:E:20:THR:HG23	1.87	0.57
1:E:29:VAL:O	1:E:36:ASP:HB2	2.05	0.57
1:F:300:THR:HG22	1:F:301:ASN:N	2.15	0.57
1:B:56:VAL:HG11	1:B:116:PHE:HB2	1.85	0.57
1:C:331:VAL:O	1:C:334:GLY:N	2.37	0.57
1:D:32:LEU:HD11	1:D:176:PRO:HB3	1.86	0.57
1:A:255:VAL:HG23	1:A:289:LEU:HD11	1.85	0.57
1:B:81:PHE:CZ	1:B:83:ALA:HB2	2.40	0.57
1:B:224:ASN:HD22	1:B:264:VAL:HG22	1.70	0.57
1:E:10:PHE:CZ	1:E:26:ARG:HG3	2.39	0.57
1:B:41:VAL:HG22	1:B:105:LEU:HD13	1.87	0.57
1:C:238:ARG:HG2	1:C:238:ARG:NH1	2.15	0.57
1:E:16:ASN:OD1	1:F:267:SER:CA	2.52	0.57
1:E:148:ARG:HA	1:E:165:VAL:O	2.04	0.57
1:F:69:LEU:HA	1:F:72:LEU:HD12	1.86	0.56
1:B:331:VAL:O	1:B:334:GLY:N	2.34	0.56
1:C:170:ARG:HH21	1:C:172:VAL:HG11	1.69	0.56
1:D:270:PHE:HA	1:F:349:LYS:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LYS:HA	1:C:21:VAL:O	2.05	0.56
1:C:30:ASP:HB2	1:C:171:LYS:HG2	1.88	0.56
1:C:54:VAL:HG12	1:C:87:ALA:HB3	1.87	0.56
1:C:56:VAL:HG11	1:C:116:PHE:HB2	1.86	0.56
1:C:110:GLY:C	1:C:112:HIS:H	2.13	0.56
1:D:242:ASP:O	1:D:319:ILE:HA	2.05	0.56
1:E:96:ARG:O	1:E:98:PRO:HD3	2.05	0.56
1:F:189:ARG:HD3	1:F:337:VAL:HG11	1.87	0.56
1:F:261:ASP:O	1:F:263:GLN:NE2	2.38	0.56
1:A:62:PHE:CE1	1:A:64:TYR:HD1	2.24	0.56
1:A:333:ARG:HH21	2:Y:344:ILE:HD11	1.70	0.56
1:D:207:LYS:NZ	3:D:407:HOH:O	2.36	0.56
1:F:185:ALA:O	1:F:202:GLU:HA	2.06	0.56
1:B:63:ARG:O	1:B:141:CYS:HA	2.05	0.56
1:D:155:ILE:HG22	1:D:156:GLU:H	1.69	0.56
1:A:173:GLN:HE22	1:A:307:ILE:HG22	1.70	0.56
1:D:192:LEU:HD13	1:D:192:LEU:O	2.05	0.56
1:F:10:PHE:CZ	1:F:26:ARG:HG3	2.41	0.56
1:D:146:GLU:HG2	1:D:168:ILE:HG22	1.88	0.56
1:F:90:PRO:HG3	1:F:114:HIS:CE1	2.40	0.56
1:D:28:PHE:HB3	1:D:36:ASP:HB3	1.88	0.56
1:D:270:PHE:HA	1:F:349:LYS:HD2	1.87	0.56
1:E:344:VAL:HG12	1:E:346:MET:HG3	1.87	0.56
1:F:207:LYS:HB2	1:F:210:TYR:CE1	2.41	0.56
1:E:71:VAL:HG13	2:Y:333:LYS:HA	1.87	0.56
1:E:76:PHE:CG	1:E:77:ARG:N	2.74	0.56
1:A:49:LEU:HD11	1:A:54:VAL:HG23	1.88	0.56
1:A:29:VAL:O	1:A:36:ASP:HB2	2.06	0.55
1:B:155:ILE:HG22	1:B:156:GLU:H	1.71	0.55
1:C:200:HIS:HB2	1:C:223:THR:CG2	2.36	0.55
1:B:202:GLU:HB3	1:B:221:HIS:HB2	1.88	0.55
1:C:44:VAL:HG11	1:C:49:LEU:HD22	1.89	0.55
1:A:129:THR:HG22	1:A:142:GLY:HA3	1.87	0.55
1:B:100:ARG:CZ	1:E:259:GLU:HG2	2.35	0.55
1:B:258:LEU:HD12	1:B:276:ILE:HA	1.88	0.55
1:D:14:SER:HB3	1:D:165:VAL:HG22	1.88	0.55
1:D:242:ASP:HB2	1:E:247:SER:HB2	1.87	0.55
1:A:191:PHE:HE1	1:B:134:PRO:HA	1.71	0.55
1:A:248:THR:HG21	1:B:247:SER:HA	1.89	0.55
1:C:188:THR:HG22	1:C:200:HIS:CE1	2.41	0.55
1:A:201:LEU:HD21	1:A:220:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:HIS:HE1	1:B:162:ARG:HB3	1.71	0.55
1:E:51:ASP:HA	1:E:53:LYS:NZ	2.22	0.55
1:E:166:ARG:HH21	2:Y:339:GLY:H	1.53	0.55
1:F:189:ARG:NH1	3:F:408:HOH:O	2.39	0.55
1:B:232:LYS:HB2	1:B:330:VAL:HB	1.89	0.55
1:B:243:ILE:HA	1:B:319:ILE:HA	1.88	0.55
1:F:189:ARG:NH2	1:F:338:SER:O	2.39	0.55
1:A:26:ARG:HB2	1:A:295:LEU:HD13	1.89	0.55
1:A:43:LEU:HD22	1:A:109:LEU:HD22	1.89	0.55
1:A:270:PHE:HD1	1:C:349:LYS:HB3	1.71	0.55
1:A:272:LYS:NZ	1:A:273:VAL:O	2.36	0.55
1:B:29:VAL:HG22	1:E:277:THR:OG1	2.06	0.55
1:E:124:LEU:O	1:E:171:LYS:NZ	2.40	0.55
1:E:130:LEU:HD22	1:E:319:ILE:HD13	1.87	0.55
1:E:206:ASP:OD1	1:E:206:ASP:N	2.40	0.55
1:A:266:PRO:C	1:C:32:LEU:HD13	2.31	0.55
1:B:198:SER:O	1:B:199:LEU:HB2	2.06	0.55
1:C:212:HIS:HE1	1:C:302:LEU:HB2	1.72	0.55
1:D:201:LEU:CD2	1:D:220:VAL:HG23	2.37	0.55
1:D:210:TYR:HD1	1:D:214:GLU:HG3	1.72	0.55
1:E:15:PRO:CB	1:F:223:THR:HG22	2.37	0.55
1:E:18:LYS:HE2	1:E:49:LEU:HD12	1.89	0.55
1:D:25:LYS:NZ	1:D:36:ASP:OD2	2.27	0.55
1:E:212:HIS:CE1	1:E:301:ASN:HD22	2.25	0.55
1:B:279:LEU:HD21	1:E:27:ASP:HB2	1.89	0.54
1:C:238:ARG:CZ	1:C:326:LYS:HD3	2.36	0.54
1:D:26:ARG:NH1	2:X:341:TPO:O1P	2.25	0.54
1:D:250:GLN:HB2	1:E:248:THR:O	2.07	0.54
1:D:289:LEU:HD21	1:D:302:LEU:HD22	1.89	0.54
1:A:53:LYS:HG3	1:A:89:PRO:HG3	1.89	0.54
1:A:174:PHE:HB3	1:A:349:LYS:HB3	1.89	0.54
1:D:185:ALA:HB1	1:E:137:THR:O	2.07	0.54
1:D:242:ASP:HB3	1:D:320:LEU:HB2	1.89	0.54
1:C:128:VAL:HG13	1:C:319:ILE:HB	1.88	0.54
1:D:295:LEU:C	1:D:296:LYS:HE3	2.32	0.54
1:E:244:CYS:SG	1:E:248:THR:OG1	2.37	0.54
1:A:88:PHE:HA	1:A:114:HIS:CD2	2.43	0.54
1:D:223:THR:HG23	1:D:269:THR:HG22	1.89	0.54
1:A:175:ALA:HA	1:A:346:MET:HE2	1.89	0.54
1:A:187:THR:OG1	1:B:138:GLY:HA3	2.08	0.54
2:U:338:TPO:OG1	2:U:339:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYS:NZ	1:C:214:GLU:OE1	2.39	0.54
1:C:328:LYS:HA	1:C:338:SER:HB2	1.90	0.54
1:D:235:VAL:HG21	1:D:274:TYR:HB3	1.89	0.54
1:B:242:ASP:CG	1:B:248:THR:HG23	2.32	0.54
1:D:258:LEU:HD12	1:D:276:ILE:HA	1.89	0.54
1:C:211:TYR:HB3	1:C:348:PRO:HD3	1.88	0.54
1:C:324:ARG:HD3	1:C:341:LEU:C	2.32	0.54
1:D:186:GLU:N	1:E:137:THR:O	2.41	0.54
1:E:162:ARG:HG2	1:F:268:SER:HB3	1.89	0.54
1:D:77:ARG:C	1:D:78:LYS:HE2	2.33	0.54
1:D:186:GLU:HB2	1:D:202:GLU:HA	1.90	0.54
1:A:29:VAL:HG13	1:A:174:PHE:CE2	2.43	0.54
1:B:31:HIS:CE1	1:E:275:THR:HB	2.43	0.54
1:B:166:ARG:NE	2:V:338:TPO:HB	2.15	0.54
1:E:41:VAL:HG22	1:E:105:LEU:HD13	1.90	0.54
1:E:239:GLN:HG3	1:E:323:TYR:CE1	2.43	0.54
1:A:230:VAL:HG13	1:A:331:VAL:HG22	1.88	0.54
1:E:135:GLU:HG2	1:E:136:ASP:H	1.73	0.54
1:E:151:CYS:H	1:E:163:ASN:CG	2.16	0.54
1:A:66:ARG:HD3	1:A:138:GLY:O	2.06	0.53
1:A:187:THR:OG1	1:A:188:THR:N	2.41	0.53
1:A:296:LYS:HG2	2:U:341:TPO:OG1	2.08	0.53
1:E:202:GLU:HB3	1:E:221:HIS:HB2	1.90	0.53
1:F:25:LYS:HD3	1:F:27:ASP:O	2.08	0.53
1:F:231:LYS:HB3	1:F:330:VAL:CG2	2.36	0.53
1:C:23:LEU:HD21	1:C:147:ILE:HD13	1.91	0.53
1:D:12:LYS:NZ	1:D:166:ARG:O	2.41	0.53
1:F:49:LEU:HD11	1:F:54:VAL:HG23	1.90	0.53
1:A:193:MET:HE1	2:Y:342:LYS:HB3	1.90	0.53
1:A:265:SER:HB3	1:C:32:LEU:HB2	1.91	0.53
1:A:265:SER:HB3	1:C:33:ASP:H	1.73	0.53
1:C:240:TYR:OH	1:C:340:GLU:OE1	2.25	0.53
1:C:238:ARG:HH21	1:C:326:LYS:HD3	1.74	0.53
1:D:310:GLU:CG	1:E:74:LEU:HD21	2.39	0.53
1:E:194:SER:HB2	1:E:228:LYS:HE2	1.89	0.53
1:E:216:LEU:HB2	1:E:276:ILE:O	2.07	0.53
1:E:255:VAL:HB	1:E:289:LEU:HD11	1.90	0.53
1:F:314:LYS:NZ	3:F:411:HOH:O	2.41	0.53
1:B:130:LEU:HG	1:B:319:ILE:HD13	1.89	0.53
1:D:198:SER:O	1:D:199:LEU:HG	2.08	0.53
1:E:242:ASP:HB3	1:E:320:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:LYS:O	1:F:44:VAL:HA	2.09	0.53
1:F:91:MET:CG	1:F:92:PRO:HD3	2.17	0.53
1:A:53:LYS:CG	1:A:89:PRO:HG3	2.38	0.53
1:A:130:LEU:HD22	1:A:319:ILE:HD11	1.90	0.53
1:F:292:ASP:OD2	1:F:301:ASN:ND2	2.42	0.53
1:A:338:SER:N	1:B:287:ARG:HD2	2.24	0.53
1:E:242:ASP:O	1:E:319:ILE:HA	2.09	0.53
1:F:232:LYS:HE3	1:F:233:ILE:H	1.72	0.53
1:B:148:ARG:HG2	1:B:166:ARG:HA	1.91	0.53
1:D:242:ASP:OD1	1:D:243:ILE:N	2.42	0.53
1:E:123:ASN:OD1	1:E:123:ASN:N	2.42	0.53
1:F:207:LYS:HD3	1:F:210:TYR:OH	2.08	0.53
2:W:340:LEU:HB3	2:W:341:TPO:O	2.08	0.53
1:B:244:CYS:HB2	1:B:318:GLY:H	1.74	0.52
1:C:338:SER:OG	1:C:339:VAL:N	2.42	0.52
1:F:96:ARG:O	1:F:98:PRO:HD3	2.09	0.52
1:A:148:ARG:HE	1:A:166:ARG:HA	1.73	0.52
1:E:18:LYS:HZ1	1:E:48:TYR:HE2	1.55	0.52
1:E:145:PHE:CZ	1:E:171:LYS:HD3	2.44	0.52
1:E:313:ASN:OD1	1:E:313:ASN:N	2.40	0.52
1:A:234:ARG:NH2	1:A:257:GLN:HG3	2.23	0.52
1:B:37:PRO:HB2	1:B:117:PHE:CE1	2.43	0.52
1:B:57:THR:HG22	1:B:84:THR:HG22	1.91	0.52
1:E:95:PRO:HG3	1:E:115:PRO:HG3	1.91	0.52
1:E:264:VAL:HG12	1:E:270:PHE:HD2	1.74	0.52
1:C:150:PHE:HB2	1:C:163:ASN:ND2	2.25	0.52
1:C:295:LEU:O	1:C:298:GLU:HG2	2.10	0.52
1:E:243:ILE:HD12	1:E:251:TYR:CE2	2.44	0.52
1:A:250:GLN:HG3	1:B:247:SER:HB2	1.90	0.52
1:D:174:PHE:HD2	1:D:348:PRO:C	2.18	0.52
1:A:41:VAL:HG22	1:A:105:LEU:HD13	1.91	0.52
1:A:250:GLN:HG3	1:B:247:SER:CB	2.39	0.52
1:A:339:VAL:HG22	1:A:340:GLU:H	1.75	0.52
1:B:71:VAL:HG13	2:V:333:LYS:HB2	1.90	0.52
1:F:200:HIS:ND1	3:F:403:HOH:O	2.34	0.52
1:A:315:GLU:OE2	1:B:314:LYS:HD3	2.10	0.52
1:C:77:ARG:HE	1:C:77:ARG:N	2.07	0.52
1:D:111:GLN:NE2	3:D:402:HOH:O	2.23	0.52
1:E:96:ARG:HD3	1:E:96:ARG:C	2.35	0.52
1:A:155:ILE:HG22	1:A:156:GLU:H	1.74	0.52
1:B:206:ASP:HB2	1:E:177:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HE2	1:B:259:GLU:OE1	2.10	0.52
1:F:25:LYS:NZ	1:F:36:ASP:OD2	2.37	0.52
1:F:232:LYS:CE	1:F:233:ILE:H	2.23	0.52
1:D:324:ARG:HD3	1:D:341:LEU:C	2.35	0.52
1:E:195:ASP:OD1	1:E:195:ASP:N	2.41	0.52
1:C:326:LYS:HG3	1:C:338:SER:OG	2.10	0.51
1:E:86:GLN:NE2	1:E:156:GLU:OE1	2.39	0.51
1:D:337:VAL:HG21	1:E:135:GLU:N	2.25	0.51
1:F:207:LYS:HD3	1:F:210:TYR:CZ	2.45	0.51
1:C:343:PHE:CZ	1:C:345:LEU:HD11	2.45	0.51
1:D:207:LYS:HB2	1:D:210:TYR:CZ	2.44	0.51
1:A:237:VAL:HG22	1:A:325:VAL:HG22	1.92	0.51
1:B:238:ARG:HD2	1:B:326:LYS:HD3	1.92	0.51
1:C:174:PHE:CD2	1:C:347:HIS:HB3	2.46	0.51
1:D:12:LYS:HD2	2:X:341:TPO:O3P	2.10	0.51
1:D:22:TYR:HB2	1:D:41:VAL:HG22	1.92	0.51
1:D:232:LYS:HD2	1:D:260:GLN:O	2.10	0.51
1:E:234:ARG:NH1	3:E:413:HOH:O	2.38	0.51
1:B:324:ARG:NH1	1:B:343:PHE:HB3	2.25	0.51
1:C:76:PHE:CG	1:C:77:ARG:N	2.78	0.51
1:C:225:ASN:ND2	1:C:230:VAL:HG11	2.26	0.51
1:D:29:VAL:O	1:D:36:ASP:HB2	2.11	0.51
1:D:248:THR:CG2	1:E:248:THR:H	2.23	0.51
1:F:128:VAL:HG21	1:F:321:VAL:HG23	1.92	0.51
1:A:124:LEU:HD23	1:A:145:PHE:CE2	2.45	0.51
1:A:134:PRO:HD3	1:A:287:ARG:HD2	1.92	0.51
1:B:160:HIS:CE1	1:B:162:ARG:HB3	2.45	0.51
1:F:80:LEU:HD12	1:F:124:LEU:HG	1.93	0.51
1:D:52:ARG:CZ	1:D:53:LYS:H	2.24	0.51
1:D:240:TYR:OH	1:D:340:GLU:OE2	2.13	0.51
1:A:44:VAL:HG23	1:A:112:HIS:CD2	2.45	0.51
1:A:328:LYS:CA	1:A:338:SER:HB2	2.39	0.51
1:D:60:CYS:HB3	1:D:81:PHE:HB3	1.92	0.51
1:D:197:ARG:CG	1:D:225:ASN:HD21	2.19	0.51
1:E:23:LEU:HD22	1:E:167:LEU:HD22	1.93	0.51
1:F:12:LYS:HD2	2:Z:341:TPO:O3P	2.07	0.51
1:F:324:ARG:NH1	1:F:343:PHE:HB3	2.25	0.51
1:A:233:ILE:HG23	1:A:274:TYR:HE2	1.76	0.51
1:B:81:PHE:HZ	1:B:83:ALA:HB2	1.74	0.51
1:C:130:LEU:HG	1:C:243:ILE:HD11	1.93	0.51
1:C:232:LYS:HG3	1:C:233:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:THR:HG23	1:D:150:PHE:HE1	1.76	0.51
1:E:168:ILE:HD13	1:E:295:LEU:HB3	1.92	0.51
1:A:10:PHE:CZ	1:A:26:ARG:HG3	2.46	0.51
1:A:193:MET:HE3	2:Y:343:LEU:HB2	1.93	0.51
1:F:54:VAL:HB	1:F:88:PHE:HB3	1.93	0.51
1:F:196:ARG:HB3	1:F:225:ASN:HD22	1.76	0.51
1:B:215:PRO:HG3	1:E:174:PHE:CD2	2.46	0.50
1:D:338:SER:H	1:E:287:ARG:HD2	1.76	0.50
1:A:23:LEU:CD2	1:A:147:ILE:HD11	2.39	0.50
1:B:214:GLU:OE2	1:E:175:ALA:HB3	2.12	0.50
1:D:166:ARG:NH2	2:X:339:GLY:H	2.09	0.50
1:D:248:THR:HG22	1:E:248:THR:H	1.76	0.50
1:F:155:ILE:O	1:F:157:GLU:N	2.44	0.50
1:F:324:ARG:HD3	1:F:341:LEU:O	2.11	0.50
1:A:166:ARG:NH1	2:U:338:TPO:O1P	2.36	0.50
1:B:14:SER:HB2	1:B:165:VAL:HG22	1.92	0.50
1:C:18:LYS:O	1:C:44:VAL:HA	2.10	0.50
1:C:238:ARG:NH2	1:C:326:LYS:HD3	2.26	0.50
1:E:17:CYS:HB2	1:F:225:ASN:OD1	2.12	0.50
1:F:124:LEU:HD23	1:F:145:PHE:HE2	1.76	0.50
1:B:64:TYR:H	1:B:77:ARG:NH1	2.06	0.50
1:B:223:THR:HG23	1:B:269:THR:HG22	1.93	0.50
1:C:225:ASN:HB2	1:C:230:VAL:CG1	2.41	0.50
1:A:39:ASP:OD1	1:A:39:ASP:N	2.42	0.50
1:B:15:PRO:HB3	1:C:223:THR:OG1	2.11	0.50
1:C:189:ARG:HD3	1:C:337:VAL:HG11	1.93	0.50
1:C:230:VAL:HA	1:C:331:VAL:HA	1.94	0.50
1:D:104:ARG:NH2	3:D:413:HOH:O	2.44	0.50
1:E:21:VAL:HG22	1:E:42:VAL:HG22	1.94	0.50
1:F:234:ARG:HG3	1:F:259:GLU:HB3	1.92	0.50
1:E:200:HIS:CB	1:E:223:THR:HB	2.41	0.50
1:F:157:GLU:O	1:F:158:LYS:HE2	2.12	0.50
1:F:206:ASP:OD1	1:F:207:LYS:N	2.45	0.50
1:A:337:VAL:HA	1:B:287:ARG:HD2	1.93	0.50
1:B:72:LEU:HD12	1:B:72:LEU:O	2.12	0.50
1:B:91:MET:HG3	1:B:92:PRO:HD3	1.92	0.50
1:C:172:VAL:HG23	1:C:174:PHE:HE1	1.76	0.50
1:D:264:VAL:HG12	1:D:270:PHE:HD2	1.76	0.50
1:D:269:THR:O	1:D:269:THR:OG1	2.28	0.50
1:E:88:PHE:CD1	1:E:89:PRO:HA	2.47	0.50
1:E:102:GLN:O	1:E:106:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HE	1:C:181:PRO:HD3	1.76	0.50
1:B:225:ASN:HA	1:B:267:SER:N	2.23	0.50
1:B:296:LYS:HE3	2:V:342:LYS:HA	1.93	0.50
1:C:155:ILE:HG23	1:C:157:GLU:H	1.76	0.50
1:C:304:SER:HB2	1:C:347:HIS:CE1	2.47	0.50
1:D:240:TYR:HB3	1:D:250:GLN:HE21	1.77	0.50
1:A:66:ARG:NH1	3:A:408:HOH:O	2.44	0.49
1:A:313:ASN:OD1	1:A:313:ASN:N	2.45	0.49
1:B:187:THR:HG22	1:B:189:ARG:HG2	1.94	0.49
1:D:185:ALA:HB2	1:D:341:LEU:HD21	1.94	0.49
1:E:258:LEU:HD13	1:E:276:ILE:HG23	1.94	0.49
1:F:196:ARG:NH1	1:F:226:SER:H	2.10	0.49
1:F:232:LYS:NZ	1:F:262:ASP:O	2.45	0.49
1:A:54:VAL:HA	1:A:151:CYS:HB3	1.94	0.49
1:A:56:VAL:HG22	1:A:118:PHE:HZ	1.77	0.49
1:A:243:ILE:O	1:A:248:THR:HA	2.12	0.49
1:B:129:THR:HG23	1:B:141:CYS:O	2.12	0.49
1:C:286:LYS:HG2	1:C:287:ARG:H	1.78	0.49
1:D:41:VAL:HB	3:D:405:HOH:O	2.10	0.49
1:D:166:ARG:NH1	2:X:338:TPO:HB	2.27	0.49
1:A:252:LYS:HD3	1:B:251:TYR:HD1	1.74	0.49
1:A:305:SER:HB2	1:A:344:VAL:HG13	1.94	0.49
1:E:207:LYS:HD3	1:E:210:TYR:CE1	2.47	0.49
1:B:208:GLU:OE2	1:B:209:LEU:CD1	2.60	0.49
1:D:323:TYR:CD1	1:D:345:LEU:HD13	2.48	0.49
1:E:175:ALA:HB2	1:E:346:MET:CB	2.43	0.49
1:E:323:TYR:O	1:E:324:ARG:HD3	2.12	0.49
1:A:225:ASN:HA	1:A:267:SER:HA	1.95	0.49
1:A:242:ASP:O	1:A:319:ILE:HA	2.12	0.49
1:C:31:HIS:CE1	1:C:349:LYS:HD3	2.48	0.49
1:C:66:ARG:CB	1:C:69:LEU:HB3	2.41	0.49
1:E:14:SER:C	1:E:16:ASN:N	2.70	0.49
1:E:14:SER:C	1:E:16:ASN:H	2.19	0.49
1:C:11:LYS:HD3	1:C:22:TYR:CZ	2.47	0.49
1:C:133:GLY:HA2	1:C:287:ARG:HB2	1.94	0.49
1:C:196:ARG:NH2	1:C:198:SER:HA	2.27	0.49
1:D:310:GLU:HG3	1:E:74:LEU:HD21	1.95	0.49
1:E:242:ASP:HA	1:E:249:ALA:O	2.12	0.49
1:A:244:CYS:SG	1:A:248:THR:HG23	2.52	0.49
1:B:39:ASP:N	1:B:39:ASP:OD1	2.43	0.49
1:B:131:GLN:HB2	1:B:289:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:CYS:SG	1:B:319:ILE:HD11	2.53	0.49
1:C:23:LEU:HD13	1:C:167:LEU:HD22	1.93	0.49
1:D:331:VAL:O	1:D:334:GLY:N	2.34	0.49
1:E:52:ARG:NH2	1:E:152:ALA:O	2.45	0.49
1:C:329:LEU:O	1:C:336:ASP:HA	2.13	0.49
1:E:193:MET:HA	1:E:193:MET:HE2	1.93	0.49
1:A:238:ARG:CZ	1:A:252:LYS:HD2	2.43	0.49
1:B:59:THR:HB	1:B:82:ILE:HD12	1.95	0.49
1:C:14:SER:HB3	1:C:165:VAL:HG22	1.95	0.49
1:D:337:VAL:CG2	1:E:135:GLU:H	2.26	0.49
1:F:210:TYR:CD2	1:F:214:GLU:HB2	2.46	0.49
1:B:194:SER:HB2	1:B:228:LYS:HE2	1.95	0.49
1:B:243:ILE:O	1:B:249:ALA:N	2.46	0.49
1:E:78:LYS:HZ2	1:E:80:LEU:HD21	1.77	0.49
1:F:232:LYS:HD2	1:F:232:LYS:HA	1.48	0.49
1:A:63:ARG:HE	1:A:140:ALA:HB1	1.77	0.48
1:F:200:HIS:C	1:F:223:THR:HB	2.36	0.48
1:B:16:ASN:HD22	1:C:269:THR:CB	2.25	0.48
1:B:294:GLN:HG3	1:B:298:GLU:O	2.13	0.48
1:D:80:LEU:H	1:D:80:LEU:HD23	1.78	0.48
1:F:41:VAL:HG22	1:F:105:LEU:HD13	1.96	0.48
1:F:86:GLN:CD	1:F:91:MET:HE2	2.38	0.48
1:F:148:ARG:HA	1:F:165:VAL:O	2.14	0.48
1:F:198:SER:O	1:F:199:LEU:HG	2.13	0.48
1:A:124:LEU:HD23	1:A:145:PHE:HE2	1.78	0.48
1:B:232:LYS:NZ	1:B:261:ASP:CA	2.69	0.48
1:C:93:ASN:HB2	1:C:95:PRO:HD3	1.95	0.48
1:D:41:VAL:HG22	1:D:105:LEU:HD13	1.94	0.48
1:D:124:LEU:O	1:D:171:LYS:NZ	2.39	0.48
1:E:99:THR:HG22	1:E:101:LEU:H	1.78	0.48
1:A:122:GLN:H	1:A:122:GLN:CD	2.12	0.48
1:A:244:CYS:HB2	1:A:317:LEU:HA	1.96	0.48
1:D:185:ALA:O	1:D:202:GLU:HA	2.11	0.48
1:E:78:LYS:NZ	1:E:80:LEU:HD21	2.28	0.48
1:E:184:SER:OG	1:E:204:SER:HA	2.13	0.48
1:A:250:GLN:HG3	1:B:247:SER:OG	2.12	0.48
1:D:189:ARG:HG2	1:E:136:ASP:CG	2.38	0.48
1:A:266:PRO:HD2	1:C:33:ASP:N	2.28	0.48
1:B:126:CYS:SG	1:B:173:GLN:N	2.86	0.48
1:B:200:HIS:CB	1:B:223:THR:HB	2.37	0.48
1:C:89:PRO:O	1:C:91:MET:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:PRO:HG3	1:F:223:THR:HG23	1.95	0.48
1:E:196:ARG:H	1:E:196:ARG:HG2	1.45	0.48
1:F:264:VAL:HG13	1:F:270:PHE:HB2	1.94	0.48
1:C:226:SER:C	1:C:228:LYS:N	2.72	0.48
1:F:196:ARG:CZ	1:F:227:ALA:H	2.27	0.48
1:F:242:ASP:HB3	1:F:320:LEU:HB2	1.95	0.48
1:F:30:ASP:OD2	1:F:171:LYS:NZ	2.44	0.48
1:F:131:GLN:CB	1:F:289:LEU:H	2.25	0.48
1:F:174:PHE:HA	1:F:347:HIS:HB2	1.94	0.48
1:F:249:ALA:HB1	1:F:251:TYR:HE1	1.77	0.48
1:F:323:TYR:CG	1:F:345:LEU:HD13	2.48	0.48
2:Z:337:LYS:HD3	2:Z:337:LYS:N	2.29	0.48
1:A:184:SER:H	1:B:69:LEU:HD11	1.79	0.48
1:C:35:VAL:HG22	1:C:36:ASP:H	1.79	0.48
1:C:225:ASN:HB2	1:C:230:VAL:HG11	1.96	0.48
1:D:91:MET:O	1:D:94:PRO:HD3	2.13	0.48
1:E:129:THR:HG22	1:E:142:GLY:HA3	1.94	0.48
1:E:325:VAL:HG23	1:E:343:PHE:CE1	2.49	0.48
1:A:260:GLN:HB2	1:A:274:TYR:HE1	1.79	0.48
1:B:15:PRO:O	1:C:224:ASN:HB2	2.14	0.48
1:B:52:ARG:NH2	1:B:152:ALA:O	2.47	0.48
1:E:130:LEU:HD23	1:E:141:CYS:HB3	1.96	0.48
1:A:146:GLU:HG2	1:A:168:ILE:HA	1.96	0.47
1:D:286:LYS:HG2	1:D:287:ARG:H	1.79	0.47
1:E:30:ASP:HB2	1:E:171:LYS:HG3	1.94	0.47
1:E:62:PHE:O	1:E:77:ARG:HB3	2.14	0.47
1:F:185:ALA:HB2	1:F:341:LEU:HD21	1.96	0.47
1:D:324:ARG:HG2	1:D:341:LEU:H	1.79	0.47
1:E:168:ILE:HD12	1:E:168:ILE:O	2.14	0.47
1:F:86:GLN:NE2	1:F:156:GLU:OE1	2.37	0.47
1:F:205:LEU:HD23	1:F:218:VAL:HA	1.95	0.47
1:A:222:VAL:CG1	1:A:270:PHE:HB3	2.44	0.47
1:B:52:ARG:NH1	3:B:409:HOH:O	2.44	0.47
1:B:131:GLN:NE2	1:B:286:LYS:O	2.46	0.47
1:C:209:LEU:HA	1:C:344:VAL:O	2.15	0.47
1:F:120:ILE:HG23	1:F:124:LEU:HD22	1.95	0.47
1:A:233:ILE:HG23	1:A:233:ILE:O	2.15	0.47
2:W:342:LYS:HD2	2:W:342:LYS:O	2.14	0.47
1:D:39:ASP:N	1:D:39:ASP:OD1	2.47	0.47
1:E:126:CYS:SG	1:E:173:GLN:HG3	2.55	0.47
1:F:29:VAL:O	1:F:36:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:ASP:HA	1:F:249:ALA:O	2.15	0.47
1:B:76:PHE:CZ	1:B:77:ARG:HG2	2.49	0.47
1:B:324:ARG:NH2	1:B:325:VAL:HB	2.29	0.47
1:C:39:ASP:HB2	1:C:102:GLN:HE21	1.80	0.47
1:C:91:MET:O	1:C:92:PRO:C	2.55	0.47
1:D:74:LEU:HD13	1:D:74:LEU:O	2.14	0.47
1:D:337:VAL:HG21	1:E:134:PRO:N	2.30	0.47
1:A:258:LEU:HD12	1:A:276:ILE:HA	1.96	0.47
1:B:128:VAL:O	1:B:142:GLY:HA2	2.15	0.47
1:C:183:PRO:HG2	1:C:205:LEU:HD12	1.96	0.47
1:E:15:PRO:CG	1:F:223:THR:HG22	2.44	0.47
1:F:94:PRO:N	1:F:95:PRO:HD3	2.29	0.47
1:F:225:ASN:OD1	1:F:226:SER:OG	2.29	0.47
1:A:70:ASP:HB3	1:A:77:ARG:HH22	1.79	0.47
1:A:267:SER:HB3	1:C:32:LEU:HD22	1.96	0.47
1:A:300:THR:OG1	1:A:301:ASN:N	2.47	0.47
1:B:16:ASN:HA	1:C:224:ASN:HB2	1.95	0.47
1:B:59:THR:CB	1:B:82:ILE:HD12	2.45	0.47
1:B:211:TYR:H	1:E:211:TYR:HD2	1.61	0.47
1:B:232:LYS:HE3	1:B:233:ILE:H	1.79	0.47
1:C:151:CYS:H	1:C:163:ASN:ND2	2.12	0.47
1:C:166:ARG:HH21	2:W:339:GLY:H	1.62	0.47
1:C:207:LYS:HD3	1:C:210:TYR:CE1	2.50	0.47
1:C:240:TYR:HB2	1:C:322:SER:OG	2.15	0.47
1:C:329:LEU:N	1:C:337:VAL:O	2.47	0.47
1:E:28:PHE:CE1	1:E:38:VAL:HA	2.49	0.47
1:E:234:ARG:HA	1:E:259:GLU:HB2	1.96	0.47
1:F:205:LEU:HD11	1:F:324:ARG:HH22	1.80	0.47
1:A:48:TYR:HD1	1:A:48:TYR:O	1.98	0.47
1:A:54:VAL:HG12	1:A:87:ALA:HB3	1.95	0.47
1:B:30:ASP:OD2	1:B:171:LYS:NZ	2.47	0.47
1:B:31:HIS:ND1	1:E:275:THR:HB	2.29	0.47
1:B:107:LYS:HB3	1:B:107:LYS:HE3	1.61	0.47
1:A:193:MET:HG2	2:Y:343:LEU:HB3	1.97	0.47
1:B:130:LEU:HB2	1:B:141:CYS:HB3	1.96	0.47
1:C:12:LYS:NZ	1:C:166:ARG:O	2.47	0.47
1:E:130:LEU:HD11	1:E:243:ILE:HD11	1.97	0.47
1:F:29:VAL:CG1	1:F:349:LYS:HG2	2.45	0.47
1:A:35:VAL:HG11	1:A:120:ILE:HB	1.96	0.47
1:B:174:PHE:HB3	1:E:215:PRO:HD3	1.96	0.47
1:C:255:VAL:O	1:C:283:ASN:ND2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ARG:HD2	3:D:422:HOH:O	2.15	0.47
1:D:206:ASP:OD1	1:D:206:ASP:N	2.47	0.47
1:F:166:ARG:O	1:F:167:LEU:HB2	2.15	0.47
1:F:313:ASN:OD1	1:F:313:ASN:N	2.47	0.47
1:A:57:THR:HG23	1:A:150:PHE:HE1	1.79	0.46
1:A:101:LEU:O	1:A:105:LEU:HG	2.15	0.46
1:A:133:GLY:HA2	1:A:287:ARG:HG3	1.98	0.46
1:B:51:ASP:HA	1:B:53:LYS:NZ	2.30	0.46
1:B:57:THR:HA	1:B:83:ALA:O	2.15	0.46
1:B:206:ASP:HB2	1:E:177:GLU:HB2	1.96	0.46
1:C:81:PHE:CZ	1:C:83:ALA:HB2	2.50	0.46
1:E:18:LYS:O	1:E:44:VAL:HG12	2.14	0.46
1:E:189:ARG:HD3	1:E:337:VAL:HG11	1.95	0.46
1:F:89:PRO:O	1:F:91:MET:N	2.49	0.46
1:F:155:ILE:HG22	1:F:156:GLU:H	1.80	0.46
1:F:324:ARG:HE	1:F:325:VAL:H	1.61	0.46
1:A:130:LEU:HD11	1:A:243:ILE:CG1	2.44	0.46
1:A:197:ARG:HE	1:C:181:PRO:CD	2.28	0.46
1:A:266:PRO:HD2	1:C:33:ASP:H	1.81	0.46
1:A:295:LEU:CB	1:A:296:LYS:HZ1	2.28	0.46
1:B:277:THR:HG23	1:E:29:VAL:HG13	1.97	0.46
1:D:306:THR:OG1	1:D:320:LEU:HA	2.15	0.46
1:D:94:PRO:HB2	1:D:95:PRO:HD3	1.97	0.46
1:A:328:LYS:CE	1:A:336:ASP:HB3	2.40	0.46
1:C:300:THR:OG1	1:C:301:ASN:N	2.47	0.46
1:D:225:ASN:HA	1:D:267:SER:CA	2.44	0.46
1:D:250:GLN:CD	1:E:247:SER:HB3	2.40	0.46
1:E:216:LEU:HD13	1:E:278:PRO:HD2	1.97	0.46
1:E:223:THR:HG23	1:E:269:THR:HG22	1.96	0.46
1:F:44:VAL:CG2	1:F:49:LEU:HD13	2.41	0.46
1:F:52:ARG:NH1	1:F:153:LYS:HA	2.30	0.46
2:U:333:LYS:HG3	2:U:334:TYR:CD1	2.50	0.46
1:B:129:THR:HG22	1:B:130:LEU:O	2.15	0.46
1:D:52:ARG:NH1	1:D:153:LYS:HA	2.31	0.46
1:E:212:HIS:CD2	1:E:301:ASN:HB2	2.51	0.46
1:E:255:VAL:HG23	1:E:289:LEU:HD21	1.97	0.46
1:F:68:ASP:O	1:F:72:LEU:N	2.45	0.46
1:B:52:ARG:CZ	1:B:153:LYS:HA	2.46	0.46
1:B:186:GLU:CB	1:B:339:VAL:HG11	2.45	0.46
1:D:232:LYS:HE2	1:D:232:LYS:CA	2.35	0.46
1:F:170:ARG:NH2	3:F:407:HOH:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASP:OD1	1:A:243:ILE:N	2.48	0.46
1:B:132:PRO:HB2	1:B:137:THR:CB	2.46	0.46
1:C:201:LEU:C	1:C:201:LEU:HD13	2.41	0.46
1:D:200:HIS:O	1:D:222:VAL:HA	2.16	0.46
1:E:166:ARG:NH2	2:Y:339:GLY:H	2.13	0.46
1:F:134:PRO:CD	1:F:287:ARG:HB2	2.44	0.46
1:F:289:LEU:HB2	3:F:414:HOH:O	2.15	0.46
1:F:295:LEU:HD12	1:F:298:GLU:OE2	2.15	0.46
1:A:192:LEU:HG	1:B:284:ARG:HD3	1.98	0.46
1:A:205:LEU:HD23	1:A:218:VAL:HA	1.98	0.46
1:B:100:ARG:CZ	1:B:100:ARG:HB2	2.46	0.46
1:D:18:LYS:HZ1	1:D:49:LEU:HD12	1.81	0.46
1:D:226:SER:HB3	1:D:266:PRO:HA	1.97	0.46
1:D:228:LYS:HE3	1:E:285:GLU:OE2	2.16	0.46
1:E:130:LEU:HD22	1:E:319:ILE:HD11	1.96	0.46
1:F:56:VAL:HG11	1:F:116:PHE:HB2	1.97	0.46
1:F:292:ASP:O	1:F:300:THR:HG21	2.15	0.46
1:A:130:LEU:HD13	1:A:319:ILE:HG12	1.97	0.46
1:B:94:PRO:HD2	1:B:95:PRO:HD3	1.98	0.46
1:C:331:VAL:HG12	1:C:332:SER:H	1.81	0.46
1:D:232:LYS:NZ	1:D:262:ASP:O	2.37	0.46
1:E:17:CYS:SG	1:F:225:ASN:ND2	2.89	0.46
1:E:21:VAL:HB	3:E:462:HOH:O	2.15	0.46
1:F:92:PRO:O	1:F:93:ASN:C	2.59	0.46
1:B:28:PHE:HB3	1:B:36:ASP:HB3	1.98	0.46
1:B:208:GLU:CD	1:B:209:LEU:CD1	2.89	0.46
1:B:215:PRO:HD3	1:E:174:PHE:CG	2.51	0.46
1:B:230:VAL:HG21	1:B:264:VAL:CG1	2.46	0.46
1:B:239:GLN:HG3	1:B:323:TYR:CE1	2.51	0.46
1:B:328:LYS:HA	1:B:338:SER:HB2	1.98	0.46
1:C:53:LYS:HE3	1:C:89:PRO:HG3	1.98	0.46
2:W:339:GLY:O	2:W:340:LEU:HD23	2.16	0.46
1:D:58:LEU:HD21	1:D:169:ILE:HD11	1.96	0.46
1:F:294:GLN:HB3	1:F:300:THR:OG1	2.17	0.46
1:A:62:PHE:CD1	1:A:64:TYR:HD1	2.34	0.45
1:C:284:ARG:NH2	3:C:419:HOH:O	2.49	0.45
1:E:52:ARG:CZ	1:E:153:LYS:HA	2.46	0.45
1:E:170:ARG:NH2	1:E:294:GLN:HA	2.31	0.45
1:F:54:VAL:HG12	1:F:87:ALA:HB3	1.97	0.45
1:F:60:CYS:HB2	1:F:145:PHE:CE2	2.51	0.45
1:F:126:CYS:SG	1:F:173:GLN:HB2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:VAL:HG13	1:F:319:ILE:HB	1.97	0.45
1:F:260:GLN:HB2	1:F:274:TYR:HE1	1.80	0.45
1:A:329:LEU:HD13	1:B:135:GLU:HB3	1.98	0.45
1:B:12:LYS:HB2	2:V:341:TPO:O3P	2.16	0.45
1:B:213:GLY:HA3	1:E:211:TYR:HB3	1.97	0.45
1:C:135:GLU:HG3	1:C:136:ASP:OD1	2.17	0.45
1:F:12:LYS:HD2	2:Z:341:TPO:P	2.54	0.45
1:F:18:LYS:HE2	1:F:49:LEU:HD12	1.97	0.45
1:F:332:SER:HA	1:F:333:ARG:HA	1.66	0.45
1:A:186:GLU:HB2	1:A:202:GLU:HG3	1.97	0.45
1:C:174:PHE:HD2	1:C:348:PRO:O	1.99	0.45
1:C:234:ARG:HH12	1:C:257:GLN:HG3	1.79	0.45
1:A:28:PHE:HB3	1:A:36:ASP:HB3	1.98	0.45
1:A:122:GLN:OE1	1:A:122:GLN:N	2.35	0.45
1:A:183:PRO:HG3	1:A:208:GLU:HG2	1.99	0.45
1:A:264:VAL:HG22	1:A:265:SER:H	1.81	0.45
1:B:15:PRO:HB3	1:C:223:THR:HA	1.98	0.45
1:B:90:PRO:HB2	1:B:93:ASN:HA	1.97	0.45
1:B:116:PHE:CD1	1:B:116:PHE:C	2.94	0.45
1:B:236:SER:HA	1:B:257:GLN:CB	2.43	0.45
1:C:47:ASP:HA	1:C:50:LYS:HG2	1.98	0.45
1:D:62:PHE:CD1	1:D:318:GLY:HA2	2.51	0.45
1:F:52:ARG:C	1:F:53:LYS:HD2	2.42	0.45
1:A:197:ARG:CD	1:C:180:GLY:HA2	2.47	0.45
1:C:155:ILE:HG13	1:C:156:GLU:H	1.81	0.45
1:E:146:GLU:HG2	1:E:167:LEU:O	2.17	0.45
1:A:88:PHE:CD2	1:A:89:PRO:HD3	2.51	0.45
1:B:162:ARG:HG2	1:C:268:SER:HB3	1.98	0.45
1:E:29:VAL:HG12	1:E:31:HIS:HD2	1.81	0.45
1:E:210:TYR:CG	1:E:214:GLU:HG3	2.52	0.45
1:A:64:TYR:HB2	1:A:245:LEU:HD22	1.98	0.45
1:D:91:MET:O	1:D:92:PRO:C	2.60	0.45
1:D:91:MET:HB3	1:D:92:PRO:HD2	1.98	0.45
1:D:222:VAL:N	1:D:270:PHE:O	2.49	0.45
1:E:56:VAL:HG22	1:E:118:PHE:HZ	1.81	0.45
1:E:170:ARG:HH21	1:E:293:GLY:C	2.24	0.45
1:E:240:TYR:HD2	1:E:250:GLN:HB3	1.82	0.45
1:E:300:THR:OG1	1:E:301:ASN:N	2.50	0.45
1:A:62:PHE:CE2	1:A:318:GLY:HA2	2.52	0.45
1:B:49:LEU:HD11	1:B:54:VAL:HG23	1.97	0.45
1:B:166:ARG:NH1	1:B:166:ARG:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASN:O	1:C:16:ASN:ND2	2.39	0.45
1:D:168:ILE:HD11	1:D:296:LYS:CE	2.28	0.45
1:D:300:THR:OG1	1:D:301:ASN:N	2.50	0.45
1:E:15:PRO:HG3	1:F:223:THR:HG22	1.96	0.45
1:E:145:PHE:CE2	1:E:171:LYS:HD3	2.52	0.45
1:A:76:PHE:CE1	1:A:77:ARG:HG2	2.51	0.45
1:A:196:ARG:CZ	1:A:196:ARG:HB3	2.46	0.45
1:B:20:THR:HG22	1:B:22:TYR:CE1	2.52	0.45
1:B:166:ARG:NH2	2:V:338:TPO:HG23	2.27	0.45
1:B:174:PHE:O	1:B:346:MET:HE2	2.16	0.45
1:D:242:ASP:OD2	1:D:320:LEU:HD12	2.17	0.45
2:Y:338:TPO:HG23	2:Y:339:GLY:N	2.32	0.45
1:F:189:ARG:NH2	1:F:339:VAL:HB	2.32	0.45
1:F:196:ARG:NH2	1:F:227:ALA:HB3	2.32	0.45
1:A:197:ARG:CG	1:C:180:GLY:HA2	2.47	0.45
1:A:223:THR:HG21	1:C:209:LEU:HB2	1.99	0.45
1:C:323:TYR:HB2	1:C:345:LEU:HD13	1.98	0.45
1:D:304:SER:HB3	1:D:347:HIS:CD2	2.51	0.45
2:Z:337:LYS:HD3	2:Z:337:LYS:H	1.81	0.45
1:C:172:VAL:HG23	1:C:174:PHE:CE1	2.51	0.44
1:E:49:LEU:HG	1:E:52:ARG:O	2.17	0.44
1:A:12:LYS:HD3	1:A:166:ARG:O	2.16	0.44
1:A:71:VAL:C	1:A:73:GLY:H	2.25	0.44
1:B:19:LEU:O	1:B:165:VAL:HG21	2.16	0.44
1:B:216:LEU:O	1:B:275:THR:HA	2.18	0.44
1:C:99:THR:OG1	1:C:102:GLN:NE2	2.50	0.44
1:D:10:PHE:CE1	1:D:23:LEU:HB2	2.52	0.44
1:D:248:THR:C	1:E:248:THR:HB	2.42	0.44
1:E:94:PRO:HG2	1:E:95:PRO:HD3	1.98	0.44
1:F:232:LYS:HE3	1:F:233:ILE:O	2.17	0.44
1:B:29:VAL:HG11	1:B:31:HIS:CE1	2.52	0.44
1:C:30:ASP:HB3	1:C:173:GLN:HA	1.99	0.44
1:C:305:SER:N	1:C:345:LEU:O	2.45	0.44
1:F:60:CYS:SG	1:F:80:LEU:HB3	2.58	0.44
1:F:155:ILE:HD12	1:F:155:ILE:H	1.83	0.44
1:F:309:LYS:HG3	1:F:310:GLU:H	1.83	0.44
1:B:189:ARG:HD2	1:B:337:VAL:HG11	2.00	0.44
1:C:324:ARG:NH2	1:C:325:VAL:HB	2.31	0.44
1:D:329:LEU:HD13	1:E:135:GLU:OE1	2.16	0.44
1:A:324:ARG:HD2	1:A:324:ARG:HA	1.61	0.44
1:B:52:ARG:NH1	1:B:153:LYS:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:ASN:O	1:E:267:SER:HA	2.17	0.44
1:F:211:TYR:CE2	1:F:348:PRO:HB3	2.53	0.44
1:C:54:VAL:HA	1:C:151:CYS:HB3	2.00	0.44
1:D:240:TYR:HB3	1:D:250:GLN:NE2	2.32	0.44
1:B:18:LYS:HE2	1:B:49:LEU:HD12	2.00	0.44
1:B:324:ARG:HA	1:B:343:PHE:CD1	2.53	0.44
1:C:243:ILE:HG12	1:C:319:ILE:HG12	1.99	0.44
1:A:238:ARG:HE	1:A:326:LYS:HD3	1.82	0.44
1:C:58:LEU:HD22	1:C:146:GLU:O	2.17	0.44
1:C:150:PHE:HB3	1:C:164:SER:HA	1.99	0.44
1:C:237:VAL:HG22	1:C:325:VAL:HG22	2.00	0.44
1:C:326:LYS:HE2	1:C:328:LYS:HB2	1.99	0.44
1:D:153:LYS:HB3	1:D:153:LYS:HE3	1.73	0.44
1:F:35:VAL:CG1	1:F:120:ILE:HB	2.48	0.44
1:F:209:LEU:HG	1:F:344:VAL:HB	2.00	0.44
1:A:230:VAL:HG22	1:A:331:VAL:HG22	1.99	0.44
1:B:9:VAL:HG13	1:D:333:ARG:NH1	2.33	0.44
1:B:166:ARG:HH21	2:V:338:TPO:HB	1.81	0.44
1:C:147:ILE:HG12	1:C:167:LEU:HB3	2.00	0.44
1:D:268:SER:HB3	1:F:349:LYS:CE	2.48	0.44
1:E:189:ARG:HH12	1:E:329:LEU:HD13	1.82	0.44
1:A:62:PHE:HE2	1:A:317:LEU:C	2.26	0.43
1:C:110:GLY:C	1:C:112:HIS:N	2.76	0.43
1:D:220:VAL:O	1:D:220:VAL:HG13	2.18	0.43
1:D:310:GLU:HG2	1:E:74:LEU:HD21	2.00	0.43
1:E:175:ALA:HB1	1:E:176:PRO:HD2	2.00	0.43
1:A:234:ARG:HH21	1:A:257:GLN:HG3	1.82	0.43
1:B:60:CYS:SG	1:B:80:LEU:HD23	2.58	0.43
1:B:76:PHE:O	1:B:77:ARG:CZ	2.66	0.43
1:B:91:MET:O	1:B:94:PRO:HD3	2.18	0.43
1:F:12:LYS:HZ1	1:F:167:LEU:HA	1.83	0.43
1:F:19:LEU:HD21	1:F:151:CYS:SG	2.58	0.43
1:A:174:PHE:CB	1:A:349:LYS:HB3	2.49	0.43
1:A:264:VAL:HG22	1:A:265:SER:N	2.33	0.43
1:B:44:VAL:HG11	1:B:49:LEU:HD22	2.00	0.43
1:C:88:PHE:HD2	1:C:114:HIS:NE2	2.16	0.43
1:C:91:MET:O	1:C:93:ASN:CA	2.66	0.43
1:C:295:LEU:C	1:C:296:LYS:HG3	2.42	0.43
1:F:57:THR:HG22	1:F:84:THR:HG22	1.98	0.43
1:B:76:PHE:O	1:B:77:ARG:NH2	2.51	0.43
1:C:57:THR:HA	1:C:83:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:VAL:HG22	1:C:270:PHE:HD2	1.83	0.43
1:D:339:VAL:HG21	1:E:137:THR:N	2.33	0.43
1:E:162:ARG:HA	1:F:269:THR:N	2.32	0.43
1:F:30:ASP:HB3	1:F:173:GLN:HA	2.00	0.43
1:B:10:PHE:CZ	1:B:26:ARG:HG3	2.54	0.43
1:B:230:VAL:HG21	1:B:264:VAL:HG13	2.00	0.43
1:C:48:TYR:HD1	1:C:52:ARG:NH1	2.16	0.43
1:C:324:ARG:HA	1:C:324:ARG:HD2	1.77	0.43
1:D:243:ILE:HD12	1:D:251:TYR:CE1	2.53	0.43
1:D:272:LYS:HG3	1:D:273:VAL:N	2.33	0.43
1:A:25:LYS:NZ	1:A:36:ASP:OD2	2.39	0.43
1:A:46:PRO:HB3	1:A:112:HIS:CE1	2.54	0.43
1:A:64:TYR:CG	1:A:245:LEU:HD13	2.53	0.43
1:B:29:VAL:CG1	1:B:31:HIS:CE1	3.02	0.43
1:C:66:ARG:HB2	1:C:69:LEU:HD22	2.00	0.43
1:C:257:GLN:N	3:C:418:HOH:O	2.48	0.43
1:B:53:LYS:HE3	1:B:89:PRO:HG3	2.01	0.43
1:B:242:ASP:HA	1:B:249:ALA:O	2.19	0.43
1:C:90:PRO:HB2	1:C:93:ASN:HB3	1.99	0.43
1:C:90:PRO:O	1:C:91:MET:O	2.37	0.43
1:D:326:LYS:HE3	1:D:338:SER:HB3	2.01	0.43
1:F:11:LYS:HB3	1:F:22:TYR:CD2	2.53	0.43
1:F:185:ALA:HB2	1:F:341:LEU:HD11	2.01	0.43
1:B:222:VAL:HG11	1:B:264:VAL:HG11	2.01	0.43
1:B:231:LYS:HD2	3:B:410:HOH:O	2.19	0.43
1:C:146:GLU:CD	1:C:168:ILE:HG13	2.44	0.43
1:D:81:PHE:CG	1:D:124:LEU:HD21	2.53	0.43
1:D:304:SER:HB3	1:D:347:HIS:NE2	2.34	0.43
2:Y:341:TPO:O2P	2:Y:341:TPO:O	2.36	0.43
1:F:224:ASN:OD1	1:F:225:ASN:N	2.51	0.43
1:A:60:CYS:HB3	1:A:81:PHE:HB3	2.01	0.43
1:A:233:ILE:CG2	1:A:274:TYR:HE2	2.31	0.43
1:A:252:LYS:HD3	1:B:251:TYR:CE1	2.54	0.43
1:A:327:VAL:O	1:A:338:SER:HA	2.18	0.43
1:B:99:THR:O	1:B:103:ASP:N	2.51	0.43
1:D:52:ARG:CZ	1:D:153:LYS:HA	2.49	0.43
1:F:200:HIS:HB2	1:F:223:THR:HB	2.01	0.43
1:F:233:ILE:HG12	1:F:329:LEU:HG	2.01	0.43
1:B:131:GLN:HB3	1:B:289:LEU:H	1.83	0.43
1:B:239:GLN:NE2	1:B:290:ALA:HB3	2.33	0.43
1:C:256:ALA:HB1	3:C:418:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:LYS:HZ3	1:D:166:ARG:NH1	2.17	0.43
1:D:338:SER:H	1:E:287:ARG:CD	2.32	0.43
1:A:225:ASN:O	1:A:267:SER:HB2	2.19	0.42
1:B:240:TYR:HB2	1:B:322:SER:HB2	2.01	0.42
1:D:131:GLN:HB2	1:D:289:LEU:O	2.18	0.42
1:D:205:LEU:HD11	1:D:324:ARG:HH22	1.84	0.42
1:D:326:LYS:HD3	1:D:328:LYS:HB2	2.01	0.42
1:E:52:ARG:NH1	1:E:153:LYS:HA	2.34	0.42
1:E:54:VAL:HA	1:E:151:CYS:SG	2.58	0.42
1:E:61:ALA:HB3	1:E:144:ASP:OD1	2.19	0.42
1:E:216:LEU:HD22	1:E:278:PRO:HD3	2.00	0.42
1:A:124:LEU:HB3	1:A:145:PHE:HZ	1.84	0.42
1:A:324:ARG:HG2	1:A:341:LEU:H	1.84	0.42
1:C:67:GLU:HG3	3:W:402:HOH:O	2.19	0.42
1:C:233:ILE:HG12	1:C:329:LEU:HG	2.01	0.42
1:C:264:VAL:HG22	1:C:270:PHE:CD2	2.54	0.42
1:D:54:VAL:HA	1:D:151:CYS:SG	2.59	0.42
1:D:177:GLU:OE1	1:D:177:GLU:N	2.48	0.42
1:D:242:ASP:HB3	1:D:320:LEU:CB	2.48	0.42
1:D:266:PRO:CD	1:F:33:ASP:HB2	2.38	0.42
1:E:233:ILE:HB	1:E:274:TYR:HE2	1.84	0.42
1:A:10:PHE:CE1	1:A:23:LEU:HB2	2.54	0.42
1:B:29:VAL:HG22	1:E:277:THR:CG2	2.48	0.42
1:B:57:THR:HG23	1:B:150:PHE:HE1	1.84	0.42
1:B:324:ARG:HD3	1:B:341:LEU:O	2.19	0.42
1:C:10:PHE:CE1	1:C:23:LEU:HB2	2.54	0.42
1:D:54:VAL:HG22	1:D:151:CYS:SG	2.59	0.42
1:D:339:VAL:HG22	1:E:137:THR:HG22	2.00	0.42
2:X:333:LYS:HB2	2:X:334:TYR:H	1.62	0.42
1:E:26:ARG:HH12	2:Y:343:LEU:HD12	1.85	0.42
1:F:57:THR:OG1	1:F:150:PHE:HE2	2.02	0.42
1:A:155:ILE:O	1:A:157:GLU:N	2.52	0.42
1:A:248:THR:CG2	1:B:247:SER:HA	2.48	0.42
1:B:254:PRO:CG	1:B:257:GLN:HE22	2.33	0.42
1:D:338:SER:H	1:E:287:ARG:NE	2.17	0.42
1:F:197:ARG:H	1:F:197:ARG:HG3	1.41	0.42
1:A:19:LEU:HG	1:A:44:VAL:HG12	2.01	0.42
1:A:197:ARG:O	1:A:199:LEU:N	2.43	0.42
1:A:197:ARG:HD3	1:C:180:GLY:HA2	2.01	0.42
1:C:90:PRO:C	1:C:91:MET:O	2.63	0.42
1:C:238:ARG:NE	1:C:326:LYS:CD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:VAL:O	1:D:117:PHE:HA	2.19	0.42
1:F:57:THR:HA	1:F:83:ALA:O	2.18	0.42
1:A:11:LYS:HB3	1:A:22:TYR:CD2	2.54	0.42
1:B:324:ARG:NE	1:B:341:LEU:HB3	2.35	0.42
2:W:338:TPO:O2P	2:W:338:TPO:HG21	2.19	0.42
1:E:162:ARG:HA	1:F:269:THR:C	2.44	0.42
1:E:170:ARG:NH2	1:E:293:GLY:O	2.48	0.42
1:F:196:ARG:HG3	3:F:446:HOH:O	2.18	0.42
1:A:26:ARG:HH11	2:U:344:ILE:HD12	1.84	0.42
1:A:71:VAL:HG11	2:U:334:TYR:CE1	2.55	0.42
1:A:199:LEU:HD22	1:B:135:GLU:HG3	1.98	0.42
1:B:230:VAL:O	1:B:231:LYS:HB3	2.20	0.42
1:C:30:ASP:OD2	1:C:171:LYS:NZ	2.53	0.42
1:C:332:SER:C	1:C:334:GLY:H	2.28	0.42
1:D:148:ARG:HE	1:D:166:ARG:HB3	1.84	0.42
1:E:131:GLN:HB2	1:E:289:LEU:O	2.19	0.42
1:E:332:SER:HA	1:E:333:ARG:HA	1.75	0.42
1:F:153:LYS:HD3	3:F:459:HOH:O	2.19	0.42
1:F:344:VAL:HG11	1:F:346:MET:HE3	2.00	0.42
2:U:345:ASP:OD1	2:U:345:ASP:C	2.63	0.42
1:B:82:ILE:O	1:B:82:ILE:HG23	2.20	0.42
1:B:174:PHE:HB3	1:E:215:PRO:CD	2.50	0.42
1:C:12:LYS:HG3	2:W:341:TPO:HG21	2.02	0.42
1:D:57:THR:HG22	1:D:84:THR:HG22	2.02	0.42
1:D:224:ASN:OD1	1:D:225:ASN:N	2.53	0.42
1:E:16:ASN:OD1	1:F:267:SER:HA	2.17	0.42
1:E:124:LEU:HD23	1:E:145:PHE:CE2	2.54	0.42
1:F:10:PHE:HB2	2:Z:343:LEU:O	2.19	0.42
1:F:152:ALA:HB2	1:F:159:SER:HA	2.00	0.42
1:A:30:ASP:HB3	1:A:172:VAL:O	2.20	0.42
1:B:300:THR:OG1	1:B:301:ASN:N	2.52	0.42
1:C:44:VAL:HG12	1:C:112:HIS:CE1	2.54	0.42
1:C:200:HIS:HB2	1:C:223:THR:HG21	2.01	0.42
1:E:234:ARG:CB	1:E:328:LYS:HD2	2.46	0.42
1:E:287:ARG:HG2	1:E:288:GLY:N	2.35	0.42
1:E:310:GLU:OE1	1:E:310:GLU:N	2.52	0.42
1:F:12:LYS:CE	1:F:166:ARG:O	2.62	0.42
1:B:168:ILE:HD12	1:B:295:LEU:HD22	2.02	0.42
1:C:54:VAL:N	1:C:88:PHE:O	2.53	0.42
1:C:264:VAL:HG13	1:C:270:PHE:CB	2.46	0.42
1:D:280:LEU:HG	1:D:301:ASN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:HIS:NE2	1:E:302:LEU:O	2.48	0.42
1:E:269:THR:OG1	3:E:401:HOH:O	2.22	0.42
1:F:10:PHE:CE2	1:F:26:ARG:HG3	2.55	0.42
1:A:257:GLN:NE2	3:A:413:HOH:O	2.52	0.41
1:A:269:THR:O	1:C:349:LYS:HE3	2.20	0.41
1:A:337:VAL:HG13	1:B:133:GLY:HA3	2.01	0.41
1:D:157:GLU:O	1:D:157:GLU:CD	2.62	0.41
1:D:185:ALA:CB	1:E:137:THR:HG23	2.43	0.41
1:D:266:PRO:HD2	1:F:33:ASP:CB	2.42	0.41
1:F:86:GLN:CG	1:F:91:MET:CE	2.96	0.41
1:A:88:PHE:O	1:A:90:PRO:HD3	2.19	0.41
1:A:305:SER:N	1:A:345:LEU:O	2.43	0.41
1:A:307:ILE:HD12	1:B:246:PHE:HZ	1.85	0.41
1:B:134:PRO:HB2	1:B:135:GLU:OE1	2.20	0.41
1:B:162:ARG:HG3	1:C:270:PHE:HA	2.01	0.41
1:B:237:VAL:HG22	1:B:325:VAL:HG22	2.02	0.41
1:D:211:TYR:CG	1:D:348:PRO:HG3	2.55	0.41
1:E:118:PHE:HE2	1:E:147:ILE:HG23	1.85	0.41
1:A:26:ARG:CD	1:A:296:LYS:NZ	2.84	0.41
1:A:134:PRO:HD3	1:A:287:ARG:CD	2.51	0.41
1:A:239:GLN:NE2	1:A:290:ALA:HB3	2.35	0.41
1:A:255:VAL:O	1:A:283:ASN:ND2	2.38	0.41
1:B:202:GLU:OE2	1:B:204:SER:HB2	2.20	0.41
1:C:120:ILE:N	3:C:421:HOH:O	2.52	0.41
1:C:232:LYS:NZ	1:C:262:ASP:HB2	2.34	0.41
1:D:111:GLN:H	1:D:111:GLN:HG2	1.55	0.41
1:E:51:ASP:HA	1:E:53:LYS:HZ3	1.85	0.41
1:F:305:SER:O	1:F:346:MET:HE2	2.21	0.41
1:A:272:LYS:HG2	1:A:274:TYR:CZ	2.55	0.41
1:B:26:ARG:HA	1:B:169:ILE:HG22	2.02	0.41
1:C:96:ARG:O	1:C:98:PRO:HD3	2.21	0.41
1:C:262:ASP:OD2	1:C:274:TYR:OH	2.30	0.41
1:D:42:VAL:HG23	1:D:116:PHE:CD1	2.55	0.41
1:D:194:SER:HB3	1:D:196:ARG:NH1	2.31	0.41
1:F:66:ARG:NH1	3:F:415:HOH:O	2.49	0.41
1:A:189:ARG:HG3	1:B:134:PRO:HA	2.02	0.41
1:A:234:ARG:NH1	1:A:259:GLU:HG2	2.35	0.41
1:B:215:PRO:HD3	1:E:174:PHE:CD1	2.55	0.41
1:B:230:VAL:O	1:B:330:VAL:O	2.38	0.41
1:B:253:CYS:HB2	3:B:422:HOH:O	2.21	0.41
1:C:63:ARG:HA	1:C:77:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ARG:CZ	1:C:341:LEU:HB2	2.50	0.41
2:X:342:LYS:O	2:X:342:LYS:HD3	2.21	0.41
1:E:198:SER:O	1:E:199:LEU:HG	2.20	0.41
1:F:54:VAL:HA	1:F:151:CYS:SG	2.60	0.41
1:A:64:TYR:CG	1:A:245:LEU:CD1	3.03	0.41
1:A:242:ASP:HB3	1:A:320:LEU:N	2.34	0.41
1:A:331:VAL:O	1:A:334:GLY:N	2.35	0.41
1:B:8:ARG:HD3	1:B:8:ARG:HA	1.83	0.41
2:V:344:ILE:HD11	1:D:333:ARG:NH2	2.36	0.41
1:D:224:ASN:O	1:D:268:SER:N	2.54	0.41
1:D:324:ARG:HD2	1:D:324:ARG:HA	1.74	0.41
1:E:323:TYR:CG	1:E:345:LEU:HD13	2.56	0.41
1:A:26:ARG:NH2	2:U:341:TPO:O3P	2.51	0.41
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.85	0.41
2:U:339:GLY:O	2:U:340:LEU:HB2	2.20	0.41
1:B:234:ARG:NH1	1:E:100:ARG:NH2	2.67	0.41
1:B:277:THR:HG23	1:E:29:VAL:CG1	2.50	0.41
1:C:37:PRO:HA	3:C:421:HOH:O	2.21	0.41
1:D:174:PHE:CD2	1:D:348:PRO:C	2.98	0.41
1:D:268:SER:HB3	1:F:349:LYS:HE3	2.02	0.41
1:D:281:SER:HA	1:D:284:ARG:HB2	2.02	0.41
1:E:64:TYR:CE1	1:E:245:LEU:HD11	2.55	0.41
1:E:210:TYR:HB3	1:E:214:GLU:CD	2.45	0.41
1:F:57:THR:HG22	1:F:84:THR:HA	2.02	0.41
1:A:62:PHE:O	1:A:77:ARG:HB3	2.21	0.41
1:A:81:PHE:CZ	1:A:83:ALA:HB2	2.56	0.41
1:B:216:LEU:HD21	1:B:343:PHE:CZ	2.56	0.41
1:D:224:ASN:N	1:D:268:SER:O	2.49	0.41
1:A:30:ASP:HB2	1:A:171:LYS:HG2	2.03	0.41
1:A:224:ASN:OD1	1:A:225:ASN:N	2.54	0.41
1:A:239:GLN:HG3	1:A:323:TYR:CE2	2.56	0.41
1:A:337:VAL:CG1	1:B:133:GLY:HA3	2.51	0.41
1:B:235:VAL:HG21	1:B:274:TYR:HB3	2.03	0.41
1:B:343:PHE:CZ	1:B:345:LEU:HD11	2.56	0.41
1:C:10:PHE:CZ	1:C:26:ARG:HG3	2.56	0.41
1:D:120:ILE:HG22	1:D:121:PRO:O	2.20	0.41
1:D:226:SER:O	1:D:266:PRO:HB3	2.21	0.41
1:D:280:LEU:HD12	1:D:302:LEU:HG	2.03	0.41
1:D:307:ILE:HG12	1:D:346:MET:HE1	2.03	0.41
1:D:347:HIS:HE1	3:D:433:HOH:O	2.03	0.41
1:E:56:VAL:HG22	1:E:118:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:GLU:HG3	1:E:285:GLU:O	2.21	0.41
1:F:124:LEU:HD23	1:F:145:PHE:CE2	2.55	0.41
1:F:174:PHE:CG	1:F:347:HIS:HB2	2.56	0.41
1:B:305:SER:CB	1:B:344:VAL:HG13	2.51	0.41
1:D:86:GLN:HB3	3:D:406:HOH:O	2.20	0.41
2:X:334:TYR:N	2:X:334:TYR:CD1	2.88	0.41
1:F:324:ARG:HA	1:F:324:ARG:HD2	1.60	0.41
1:A:58:LEU:HD12	1:A:118:PHE:HB3	2.02	0.40
1:B:313:ASN:OD1	1:B:313:ASN:N	2.44	0.40
1:C:26:ARG:O	1:C:170:ARG:N	2.48	0.40
1:C:225:ASN:CG	1:C:230:VAL:HG11	2.46	0.40
1:D:100:ARG:HA	1:D:103:ASP:CB	2.44	0.40
1:D:231:LYS:HB3	1:D:330:VAL:HB	2.02	0.40
1:E:70:ASP:HB3	1:E:77:ARG:NH2	2.35	0.40
1:F:331:VAL:O	1:F:334:GLY:N	2.37	0.40
1:A:265:SER:CB	1:C:33:ASP:H	2.34	0.40
1:C:142:GLY:HA2	1:C:319:ILE:HD12	2.04	0.40
1:C:238:ARG:NH1	1:C:238:ARG:CG	2.78	0.40
1:D:242:ASP:HA	1:D:249:ALA:O	2.21	0.40
1:A:11:LYS:HB3	1:A:22:TYR:CE2	2.56	0.40
1:B:212:HIS:NE2	1:B:302:LEU:O	2.52	0.40
1:E:292:ASP:OD1	3:E:403:HOH:O	2.22	0.40
1:E:324:ARG:NH1	1:E:343:PHE:O	2.54	0.40
2:Y:343:LEU:HG	2:Y:344:ILE:H	1.85	0.40
1:A:172:VAL:HG23	1:A:174:PHE:CE2	2.57	0.40
1:A:177:GLU:H	1:A:177:GLU:CD	2.26	0.40
1:A:269:THR:HB	1:C:347:HIS:O	2.21	0.40
1:B:13:SER:HA	1:B:20:THR:CG2	2.46	0.40
1:B:235:VAL:HG23	1:B:276:ILE:HD11	2.03	0.40
1:C:131:GLN:HB2	1:C:289:LEU:O	2.20	0.40
1:C:174:PHE:HB3	1:C:349:LYS:HB2	2.03	0.40
1:C:313:ASN:OD1	1:C:313:ASN:N	2.50	0.40
1:C:330:VAL:HG13	1:C:336:ASP:OD1	2.21	0.40
1:D:58:LEU:HD11	1:D:145:PHE:HD2	1.86	0.40
1:D:239:GLN:NE2	1:D:290:ALA:HB3	2.36	0.40
1:D:241:ALA:O	1:D:250:GLN:HA	2.21	0.40
1:F:69:LEU:HA	1:F:72:LEU:HB2	2.03	0.40
1:A:149:ALA:O	1:A:164:SER:HA	2.21	0.40
1:A:233:ILE:HD11	1:A:327:VAL:HG22	2.03	0.40
1:A:266:PRO:O	1:A:267:SER:HB3	2.21	0.40
1:C:90:PRO:O	1:C:91:MET:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:VAL:HG11	1:C:225:ASN:ND2	2.37	0.40
1:C:269:THR:O	1:C:269:THR:HG22	2.21	0.40
1:C:330:VAL:HG12	1:C:334:GLY:HA2	2.03	0.40
1:D:244:CYS:SG	1:D:248:THR:HG23	2.61	0.40
1:E:124:LEU:HA	1:E:125:PRO:HD3	1.96	0.40
1:F:89:PRO:HA	1:F:90:PRO:HD3	1.89	0.40
1:F:301:ASN:N	1:F:301:ASN:OD1	2.53	0.40

All (5) 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)
1:E:197:ARG:NH2	1:F:158:LYS:NZ[1_455]	2.04	0.16
1:B:96:ARG:NH2	1:F:234:ARG:N[3_445]	2.09	0.11
1:E:197:ARG:CZ	1:F:158:LYS:NZ[1_455]	2.09	0.11
1:E:196:ARG:NH2	3:F:459:HOH:O[1_455]	2.15	0.05
1:D:349:LYS:N	1:D:349:LYS:O[2_655]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	196/377 (52%)	162 (83%)	34 (17%)	0	100	100
1	C	334/377 (89%)	270 (81%)	61 (18%)	3 (1%)	14	17
1	D	341/377 (90%)	283 (83%)	58 (17%)	0	100	100
1	E	337/377 (89%)	277 (82%)	60 (18%)	0	100	100
1	F	332/377 (88%)	280 (84%)	50 (15%)	2 (1%)	21	27
2	V	7/15 (47%)	3 (43%)	2 (29%)	2 (29%)	0	0
2	W	5/15 (33%)	3 (60%)	2 (40%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	7/15 (47%)	2 (29%)	4 (57%)	1 (14%)	0	0
2	Y	7/15 (47%)	3 (43%)	3 (43%)	1 (14%)	0	0
2	Z	5/15 (33%)	0	5 (100%)	0	100	100
All	All	1571/1960 (80%)	1283 (82%)	279 (18%)	9 (1%)	21	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	334	TYR
2	V	340	LEU
2	Y	340	LEU
1	C	92	PRO
1	C	91	MET
1	F	92	PRO
1	C	232	LYS
1	F	156	GLU
2	X	340	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/339 (91%)	308 (99%)	2 (1%)	78	89
1	B	303/339 (89%)	303 (100%)	0	100	100
1	C	306/339 (90%)	305 (100%)	1 (0%)	86	93
1	D	310/339 (91%)	309 (100%)	1 (0%)	86	93
1	E	306/339 (90%)	303 (99%)	3 (1%)	68	82
1	F	305/339 (90%)	304 (100%)	1 (0%)	86	93
2	U	8/10 (80%)	8 (100%)	0	100	100
2	V	7/10 (70%)	7 (100%)	0	100	100
2	W	5/10 (50%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	7/10 (70%)	7 (100%)	0	100	100
2	Y	7/10 (70%)	7 (100%)	0	100	100
2	Z	5/10 (50%)	4 (80%)	1 (20%)	1	1
All	All	1879/2094 (90%)	1870 (100%)	9 (0%)	81	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	GLU
1	A	346	MET
1	C	333	ARG
1	D	232	LYS
1	E	137	THR
1	E	196	ARG
1	E	208	GLU
1	F	232	LYS
2	Z	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	112	HIS
1	A	173	GLN
1	A	257	GLN
1	A	263	GLN
1	B	163	ASN
1	B	257	GLN
1	C	86	GLN
1	C	102	GLN
1	C	294	GLN
1	D	173	GLN
1	D	225	ASN
1	D	294	GLN
1	E	31	HIS
1	E	102	GLN
1	E	160	HIS
1	E	163	ASN
1	E	190	HIS
1	E	301	ASN

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Mol	Chain	Res	Type
1	F	212	HIS
1	F	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	SEP	Y	335	2	8,9,10	1.62	1 (12%)	7,12,14	1.40	2 (28%)
2	TPO	Y	341	2	8,10,11	1.72	1 (12%)	10,14,16	1.22	0
2	TPO	Y	338	2	8,10,11	1.17	0	10,14,16	1.77	1 (10%)
2	SEP	X	335	2	8,9,10	1.63	1 (12%)	7,12,14	1.83	2 (28%)
2	SEP	V	335	2	8,9,10	1.61	1 (12%)	7,12,14	1.48	2 (28%)
2	SEP	U	335	2	8,9,10	1.60	1 (12%)	7,12,14	1.31	1 (14%)
2	TPO	Z	338	2	8,10,11	1.69	1 (12%)	10,14,16	1.77	1 (10%)
2	TPO	W	341	2	8,10,11	1.66	1 (12%)	10,14,16	1.09	1 (10%)
2	TPO	X	341	2	8,10,11	1.19	0	10,14,16	1.41	2 (20%)
2	TPO	W	338	2	8,10,11	1.75	1 (12%)	10,14,16	1.33	2 (20%)
2	TPO	Z	341	2	8,10,11	1.85	3 (37%)	10,14,16	1.67	2 (20%)
2	TPO	U	341	2	8,10,11	1.72	1 (12%)	10,14,16	2.02	1 (10%)
2	TPO	X	338	2	8,10,11	1.80	1 (12%)	10,14,16	1.56	1 (10%)
2	TPO	V	338	2	8,10,11	1.82	1 (12%)	10,14,16	1.44	1 (10%)
2	TPO	V	341	1,2	8,10,11	1.20	0	10,14,16	1.58	4 (40%)
2	TPO	U	338	2	8,10,11	1.72	1 (12%)	10,14,16	2.57	2 (20%)

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	SEP	Y	335	2	-	3/6/8/10	-
2	TPO	Y	341	2	-	5/9/11/13	-
2	TPO	Y	338	2	-	6/9/11/13	-
2	SEP	X	335	2	-	3/6/8/10	-
2	SEP	V	335	2	-	5/6/8/10	-
2	SEP	U	335	2	-	2/6/8/10	-
2	TPO	Z	338	2	-	5/9/11/13	-
2	TPO	W	341	2	-	4/9/11/13	-
2	TPO	X	341	2	-	7/9/11/13	-
2	TPO	W	338	2	-	6/9/11/13	-
2	TPO	Z	341	2	-	1/9/11/13	-
2	TPO	U	341	2	-	3/9/11/13	-
2	TPO	X	338	2	-	6/9/11/13	-
2	TPO	V	338	2	-	5/9/11/13	-
2	TPO	V	341	1,2	-	4/9/11/13	-
2	TPO	U	338	2	-	3/9/11/13	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	338	TPO	P-O1P	3.67	1.61	1.50
2	Y	335	SEP	P-O1P	3.61	1.61	1.50
2	V	338	TPO	P-O1P	3.61	1.61	1.50
2	U	338	TPO	P-O1P	3.60	1.61	1.50
2	Z	338	TPO	P-O1P	3.57	1.61	1.50
2	W	341	TPO	P-O1P	3.54	1.61	1.50
2	U	335	SEP	P-O1P	3.54	1.61	1.50
2	Y	341	TPO	P-O1P	3.53	1.61	1.50
2	X	335	SEP	P-O1P	3.52	1.61	1.50
2	V	335	SEP	P-O1P	3.47	1.61	1.50
2	W	338	TPO	P-O1P	3.46	1.61	1.50
2	U	341	TPO	P-O1P	3.46	1.61	1.50
2	Z	341	TPO	P-O1P	3.33	1.60	1.50
2	Z	341	TPO	CB-CA	-2.68	1.47	1.53
2	Z	341	TPO	P-O3P	-2.10	1.47	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	338	TPO	P-OG1-CB	-6.74	105.01	123.33
2	U	341	TPO	P-OG1-CB	-5.85	107.43	123.33
2	Z	338	TPO	P-OG1-CB	-4.99	109.77	123.33
2	Y	338	TPO	P-OG1-CB	-4.47	111.19	123.33
2	Z	341	TPO	P-OG1-CB	-4.29	111.66	123.33
2	X	338	TPO	P-OG1-CB	-4.06	112.29	123.33
2	U	338	TPO	CG2-CB-CA	-3.82	105.81	113.26
2	V	338	TPO	P-OG1-CB	-3.70	113.28	123.33
2	X	335	SEP	O2P-P-OG	3.58	116.01	106.67
2	U	335	SEP	OG-CB-CA	2.81	110.88	108.14
2	Y	335	SEP	OG-P-O1P	2.72	113.79	106.44
2	X	335	SEP	OG-CB-CA	2.62	110.69	108.14
2	V	335	SEP	O2P-P-OG	2.56	113.36	106.67
2	V	341	TPO	O-C-CA	-2.53	118.26	124.77
2	W	338	TPO	P-OG1-CB	-2.52	116.48	123.33
2	V	335	SEP	OG-CB-CA	2.52	110.59	108.14
2	V	341	TPO	CG2-CB-CA	-2.45	108.48	113.26
2	X	341	TPO	P-OG1-CB	-2.40	116.81	123.33
2	V	341	TPO	P-OG1-CB	-2.25	117.22	123.33
2	X	341	TPO	O-C-CA	-2.24	119.01	124.77
2	Y	335	SEP	OG-CB-CA	2.04	110.13	108.14
2	W	338	TPO	O2P-P-OG1	2.03	113.77	105.85
2	V	341	TPO	O2P-P-OG1	2.01	113.69	105.85
2	W	341	TPO	O-C-CA	-2.01	119.60	124.77
2	Z	341	TPO	O2P-P-OG1	2.01	113.67	105.85

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	U	335	SEP	CA-CB-OG-P
2	U	338	TPO	N-CA-CB-OG1
2	U	341	TPO	N-CA-CB-OG1
2	V	335	SEP	N-CA-CB-OG
2	V	335	SEP	C-CA-CB-OG
2	V	335	SEP	CB-OG-P-O1P
2	V	338	TPO	N-CA-CB-CG2
2	V	338	TPO	N-CA-CB-OG1
2	V	338	TPO	C-CA-CB-CG2
2	V	341	TPO	N-CA-CB-CG2
2	V	341	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
2	V	341	TPO	C-CA-CB-CG2
2	V	341	TPO	CG2-CB-OG1-P
2	W	338	TPO	N-CA-CB-CG2
2	W	338	TPO	N-CA-CB-OG1
2	W	338	TPO	C-CA-CB-CG2
2	W	338	TPO	O-C-CA-CB
2	W	338	TPO	CG2-CB-OG1-P
2	W	341	TPO	N-CA-CB-OG1
2	W	341	TPO	CG2-CB-OG1-P
2	X	335	SEP	N-CA-CB-OG
2	X	335	SEP	C-CA-CB-OG
2	X	338	TPO	N-CA-CB-CG2
2	X	338	TPO	N-CA-CB-OG1
2	X	338	TPO	C-CA-CB-CG2
2	X	341	TPO	N-CA-CB-CG2
2	X	341	TPO	N-CA-CB-OG1
2	X	341	TPO	C-CA-CB-CG2
2	X	341	TPO	O-C-CA-CB
2	Y	335	SEP	N-CA-CB-OG
2	Y	335	SEP	C-CA-CB-OG
2	Y	338	TPO	N-CA-CB-OG1
2	Y	338	TPO	C-CA-CB-CG2
2	Y	341	TPO	N-CA-CB-CG2
2	Y	341	TPO	N-CA-CB-OG1
2	Y	341	TPO	CG2-CB-OG1-P
2	Z	338	TPO	N-CA-CB-CG2
2	Z	338	TPO	N-CA-CB-OG1
2	Z	338	TPO	C-CA-CB-CG2
2	Z	338	TPO	O-C-CA-CB
2	X	341	TPO	CG2-CB-OG1-P
2	Y	338	TPO	N-CA-CB-CG2
2	V	335	SEP	CB-OG-P-O3P
2	V	335	SEP	CA-CB-OG-P
2	Y	335	SEP	CA-CB-OG-P
2	U	338	TPO	C-CA-CB-CG2
2	Y	341	TPO	C-CA-CB-CG2
2	Z	338	TPO	CB-OG1-P-O1P
2	V	338	TPO	CG2-CB-OG1-P
2	X	338	TPO	CG2-CB-OG1-P
2	U	335	SEP	N-CA-CB-OG
2	U	341	TPO	CB-OG1-P-O3P
2	X	341	TPO	CB-OG1-P-O3P

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Mol	Chain	Res	Type	Atoms
2	W	338	TPO	CB-OG1-P-O1P
2	X	338	TPO	CB-OG1-P-O1P
2	X	335	SEP	CA-CB-OG-P
2	U	338	TPO	CB-OG1-P-O3P
2	U	341	TPO	O-C-CA-CB
2	V	338	TPO	O-C-CA-CB
2	W	341	TPO	O-C-CA-CB
2	X	338	TPO	O-C-CA-CB
2	Y	338	TPO	O-C-CA-CB
2	Y	341	TPO	O-C-CA-CB
2	Z	341	TPO	O-C-CA-CB
2	X	341	TPO	CB-OG1-P-O1P
2	Y	338	TPO	CB-OG1-P-O1P
2	W	341	TPO	N-CA-CB-CG2
2	Y	338	TPO	CG2-CB-OG1-P

There are no ring outliers.

13 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	341	TPO	1	0
2	Y	338	TPO	1	0
2	U	335	SEP	1	0
2	Z	338	TPO	1	0
2	W	341	TPO	3	0
2	X	341	TPO	2	0
2	W	338	TPO	1	0
2	Z	341	TPO	9	0
2	U	341	TPO	4	0
2	X	338	TPO	1	0
2	V	338	TPO	8	0
2	V	341	TPO	1	0
2	U	338	TPO	3	0

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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	343/377 (90%)	0.50	13 (3%)	44 46	14, 22, 36, 58	0
1	B	339/377 (89%)	0.53	16 (4%)	36 38	17, 23, 35, 54	0
1	C	338/377 (89%)	0.71	28 (8%)	17 19	17, 25, 41, 63	0
1	D	343/377 (90%)	0.56	17 (4%)	34 35	17, 24, 34, 46	0
1	E	339/377 (89%)	0.70	26 (7%)	19 21	17, 25, 41, 66	0
1	F	336/377 (89%)	0.57	14 (4%)	40 42	17, 24, 38, 64	0
2	U	10/15 (66%)	0.28	1 (10%)	12 14	15, 24, 30, 44	0
2	V	9/15 (60%)	1.02	1 (11%)	10 11	20, 25, 33, 35	0
2	W	7/15 (46%)	1.17	2 (28%)	1 1	22, 35, 42, 63	0
2	X	9/15 (60%)	0.99	1 (11%)	10 11	22, 31, 42, 44	0
2	Y	9/15 (60%)	1.43	2 (22%)	2 2	26, 39, 50, 75	0
2	Z	7/15 (46%)	1.82	3 (42%)	0 0	25, 37, 55, 56	0
All	All	2089/2352 (88%)	0.61	124 (5%)	28 30	14, 24, 39, 75	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	PHE	10.1
1	F	92	PRO	7.0
1	C	259	GLU	6.5
1	C	330	VAL	6.3
1	E	38	VAL	5.9
2	Y	340	LEU	5.5
1	E	96	ARG	5.5
1	E	138	GLY	5.2
1	E	73	GLY	5.1
1	C	180	GLY	4.9
1	D	92	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	332	SER	4.5
1	C	72	LEU	4.3
1	B	186	GLU	4.1
1	C	73	GLY	4.0
1	F	11	LYS	3.9
1	F	147	ILE	3.8
1	B	24	GLY	3.5
1	D	335	GLY	3.5
1	D	192	LEU	3.5
1	B	188	THR	3.5
1	F	69	LEU	3.5
1	B	137	THR	3.4
1	C	59	THR	3.4
2	Z	340	LEU	3.3
1	A	198	SER	3.3
2	V	340	LEU	3.2
1	C	71	VAL	3.2
1	A	87	ALA	3.1
1	E	240	TYR	3.1
1	B	133	GLY	3.1
2	Z	343	LEU	3.1
1	E	227	ALA	3.1
1	C	241	ALA	3.0
1	E	167	LEU	3.0
1	A	226	SER	3.0
1	E	288	GLY	3.0
1	F	163	ASN	3.0
1	F	293	GLY	3.0
2	W	339	GLY	3.0
1	B	298	GLU	2.9
1	B	14	SER	2.9
2	Y	344	ILE	2.9
1	A	163	ASN	2.9
1	B	187	THR	2.9
1	E	91	MET	2.9
1	D	347	HIS	2.8
1	A	235	VAL	2.8
1	F	159	SER	2.8
2	Z	344	ILE	2.8
1	C	70	ASP	2.8
1	C	154	SER	2.8
1	F	225	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	85	TYR	2.8
1	E	137	THR	2.7
2	U	334	TYR	2.7
1	C	199	LEU	2.7
1	E	132	PRO	2.6
1	C	61	ALA	2.6
1	E	16	ASN	2.6
1	C	325	VAL	2.6
1	C	163	ASN	2.5
1	E	40	GLY	2.5
1	F	149	ALA	2.5
1	B	185	ALA	2.5
1	D	37	PRO	2.5
1	B	184	SER	2.4
1	A	302	LEU	2.4
1	D	57	THR	2.4
1	E	119	THR	2.4
1	D	10	PHE	2.4
1	A	274	TYR	2.4
1	D	144	ASP	2.4
1	B	40	GLY	2.4
1	A	89	PRO	2.4
1	E	306	THR	2.4
1	E	204	SER	2.4
1	D	327	VAL	2.4
1	F	91	MET	2.4
1	B	213	GLY	2.3
1	B	22	TYR	2.3
1	E	220	VAL	2.3
1	A	57	THR	2.3
1	E	168	ILE	2.3
1	C	331	VAL	2.3
2	X	339	GLY	2.3
1	C	220	VAL	2.3
2	W	336	ALA	2.2
1	D	204	SER	2.2
1	D	21	VAL	2.2
1	F	62	PHE	2.2
1	F	150	PHE	2.2
1	D	196	ARG	2.2
1	B	138	GLY	2.2
1	D	40	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	334	GLY	2.2
1	E	319	ILE	2.2
1	C	201	LEU	2.2
1	E	302	LEU	2.2
1	A	42	VAL	2.2
1	D	234	ARG	2.2
1	C	181	PRO	2.2
1	B	147	ILE	2.2
1	F	128	VAL	2.2
1	C	246	PHE	2.2
1	E	299	ASP	2.1
1	A	236	SER	2.1
1	E	184	SER	2.1
1	C	236	SER	2.1
1	C	47	ASP	2.1
1	D	251	TYR	2.1
1	C	90	PRO	2.1
1	D	38	VAL	2.1
1	C	49	LEU	2.1
1	E	39	ASP	2.1
1	E	95	PRO	2.1
1	D	188	THR	2.0
1	B	152	ALA	2.0
1	C	74	LEU	2.0
1	C	48	TYR	2.0
1	C	211	TYR	2.0
1	A	166	ARG	2.0
1	C	334	GLY	2.0
1	F	152	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPO	Z	341	11/12	0.72	0.18	26,34,46,50	0
2	TPO	Y	341	11/12	0.77	0.21	45,57,68,69	0
2	TPO	W	338	11/12	0.85	0.15	44,64,75,79	0
2	TPO	X	341	11/12	0.86	0.17	47,61,64,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPO	U	338	11/12	0.89	0.15	15,26,40,43	0
2	TPO	W	341	11/12	0.90	0.12	25,29,37,48	0
2	TPO	Z	338	11/12	0.90	0.11	40,45,58,60	0
2	SEP	Y	335	10/11	0.90	0.12	29,40,46,47	0
2	TPO	V	341	11/12	0.91	0.15	16,25,41,44	0
2	TPO	X	338	11/12	0.91	0.11	30,34,40,41	0
2	TPO	Y	338	11/12	0.91	0.11	32,40,49,49	0
2	SEP	X	335	10/11	0.92	0.09	24,31,36,41	0
2	TPO	U	341	11/12	0.92	0.11	15,18,28,29	0
2	TPO	V	338	11/12	0.95	0.10	23,31,34,36	0
2	SEP	V	335	10/11	0.96	0.07	16,25,27,28	0
2	SEP	U	335	10/11	0.97	0.07	15,20,26,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.