



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 03:55 PM EDT

PDB ID : 4OR5  
Title : Crystal structure of HIV-1 Tat complexed with human P-TEFb and AFF4  
Authors : Gu, J.; Babayeva, N.D.; Suwa, Y.; Baranovskiy, A.G.; Price, D.H.; Tahirov, T.H.  
Deposited on : 2014-02-10  
Resolution : 2.90 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

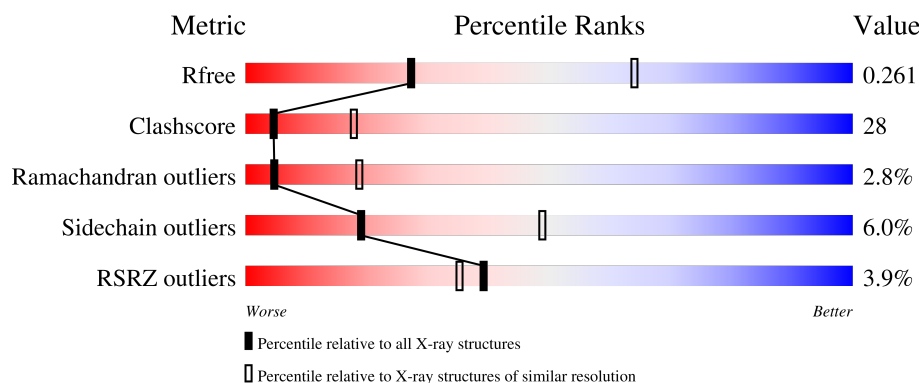
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	326	<div> <div>5%</div> <div>50%</div> <div>43%</div> <div>...</div> </div>
1	F	326	<div> <div>6%</div> <div>51%</div> <div>44%</div> <div>.</div> </div>
2	B	266	<div> <div>2%</div> <div>49%</div> <div>42%</div> <div>...</div> </div>
2	G	266	<div> <div>3%</div> <div>46%</div> <div>45%</div> <div>...</div> </div>
3	C	48	<div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	48	
4	E	43	
4	J	43	

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
5	YT3	B	303	-	-	X	-
5	YT3	E	101	-	-	X	-
6	SO4	B	304	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10895 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 Cyclin-dependent kinase 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	P	S	0	0	0
			2582	1654	447	465	1	15			
1	F	325	Total	C	N	O	P	S	0	0	0
			2628	1682	456	473	1	16			

- Molecule 2 is a protein called Cyclin-T1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S		0	0	0
			2094	1338	363	383	10				
2	G	255	Total	C	N	O	S		0	0	0
			2085	1333	362	380	10				

- Molecule 3 is a protein called Protein Tat.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	48	Total	C	N	O	S		0	0	0
			375	238	64	65	8				
3	H	48	Total	C	N	O	S		0	0	0
			375	238	64	65	8				

- Molecule 4 is a protein called AF4/FMR2 family member 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	38	Total	C	N	O	S		0	0	0
			308	193	50	63	2				
4	J	38	Total	C	N	O	S		0	0	0
			308	193	50	63	2				

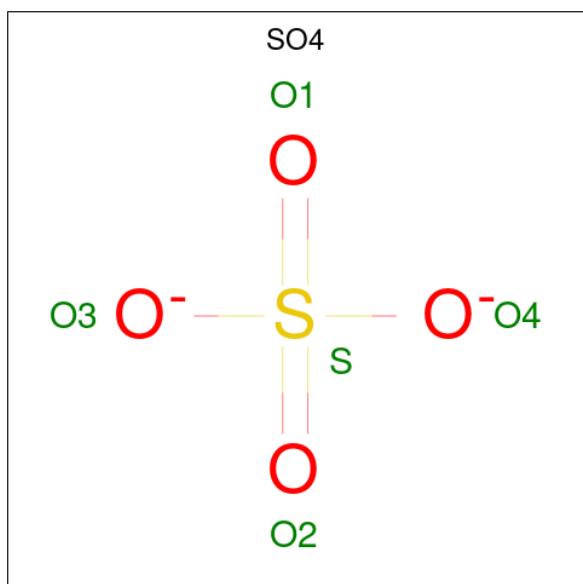
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	27	GLU	-	EXPRESSION TAG	UNP Q9UHB7
E	28	GLN	-	EXPRESSION TAG	UNP Q9UHB7
E	29	ILE	-	EXPRESSION TAG	UNP Q9UHB7
E	30	GLY	-	EXPRESSION TAG	UNP Q9UHB7
E	31	GLY	-	EXPRESSION TAG	UNP Q9UHB7
J	27	GLU	-	EXPRESSION TAG	UNP Q9UHB7
J	28	GLN	-	EXPRESSION TAG	UNP Q9UHB7
J	29	ILE	-	EXPRESSION TAG	UNP Q9UHB7
J	30	GLY	-	EXPRESSION TAG	UNP Q9UHB7
J	31	GLY	-	EXPRESSION TAG	UNP Q9UHB7

- Molecule 5 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Y 3 3	0	0
5	B	3	Total Y 3 3	0	0
5	E	2	Total Y 2 2	0	0
5	F	4	Total Y 4 4	0	0
5	G	3	Total Y 3 3	0	0
5	J	1	Total Y 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	2	Total Zn 2 2	0	0
7	H	2	Total Zn 2 2	0	0

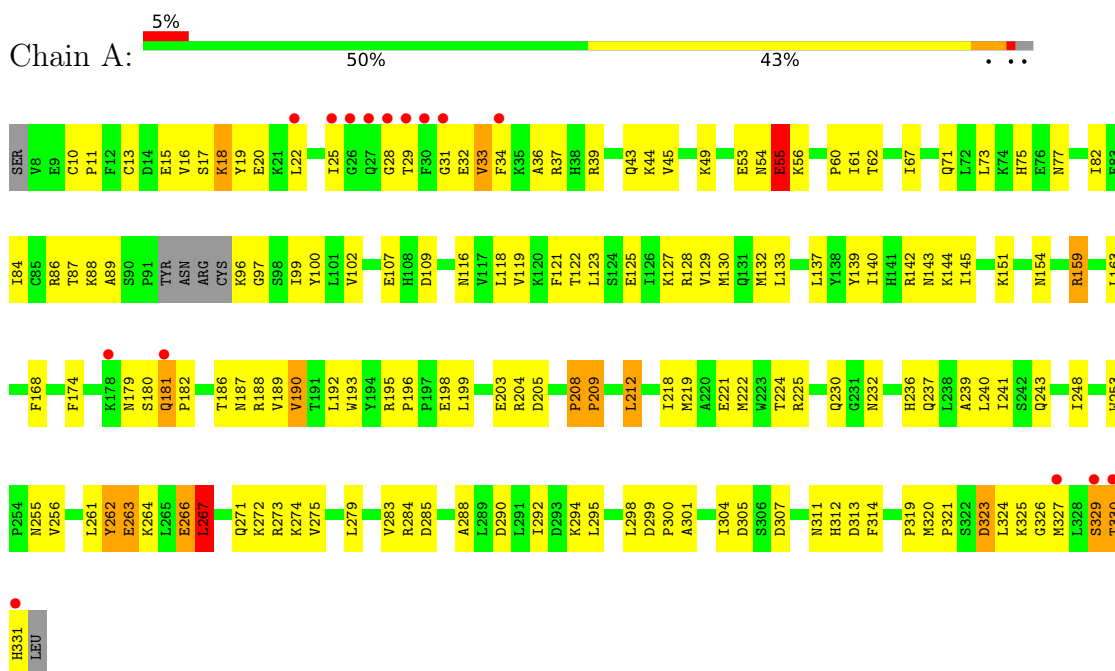
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	32	Total O 32 32	0	0
8	B	21	Total O 21 21	0	0
8	C	5	Total O 5 5	0	0
8	E	2	Total O 2 2	0	0
8	F	19	Total O 19 19	0	0
8	G	17	Total O 17 17	0	0
8	H	2	Total O 2 2	0	0
8	J	2	Total O 2 2	0	0

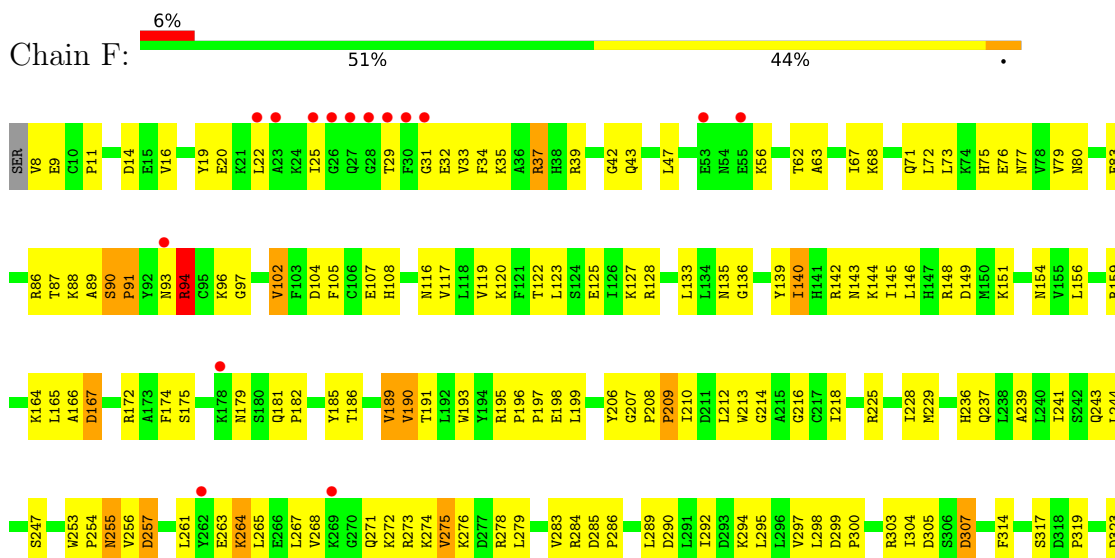
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Cyclin-dependent kinase 9

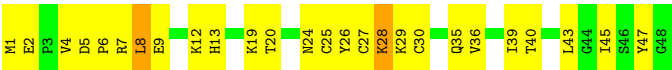


#### • Molecule 1: Cyclin-dependent kinase 9





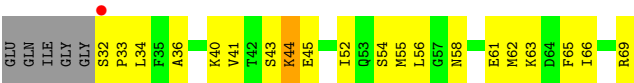




● Molecule 4: AF4/FMR2 family member 4



● Molecule 4: AF4/FMR2 family member 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.86Å 186.74Å 108.66Å 90.00° 120.24° 90.00°	Depositor
Resolution (Å)	41.90 – 2.90 41.90 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.8 (41.90-2.90) 94.7 (41.90-2.79)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	83.58 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.267 0.222 , 0.261	Depositor DCC
$R_{free}$ test set	3444 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, TPO, SO4, YT3

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	0.44	0/2623	0.69	1/3539 (0.0%)
1	F	0.40	0/2671	0.64	0/3604
2	B	0.49	0/2148	0.71	1/2927 (0.0%)
2	G	0.47	0/2139	0.69	1/2915 (0.0%)
3	C	0.52	0/387	0.65	0/522
3	H	0.52	0/387	0.63	0/522
4	E	0.50	0/313	0.72	0/416
4	J	0.42	0/313	0.71	0/416
All	All	0.45	0/10981	0.68	3/14861 (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	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	257	ASN	N-CA-C	5.36	125.47	111.00
1	A	267	LEU	CA-CB-CG	-5.34	103.02	115.30
2	B	258	TRP	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	19	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2582	0	2637	170	3
1	F	2628	0	2682	131	0
2	B	2094	0	2066	127	3
2	G	2085	0	2060	151	1
3	C	375	0	363	15	0
3	H	375	0	363	36	0
4	E	308	0	300	18	0
4	J	308	0	300	25	0
5	A	3	0	0	0	1
5	B	3	0	0	0	3
5	E	2	0	0	0	2
5	F	4	0	0	0	2
5	G	3	0	0	0	1
5	J	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	2	0
6	F	5	0	0	0	0
6	G	5	0	0	0	0
7	C	2	0	0	0	0
7	H	2	0	0	0	0
8	A	32	0	0	4	0
8	B	21	0	0	1	0
8	C	5	0	0	1	0
8	E	2	0	0	0	0
8	F	19	0	0	4	0
8	G	17	0	0	5	0
8	H	2	0	0	0	0
8	J	2	0	0	0	0
All	All	10895	0	10771	608	8

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 28.

All (608) 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)
2:B:118:LEU:HD12	2:B:118:LEU:H	1.04	1.13
2:G:16:ARG:HH11	2:G:16:ARG:HB3	1.04	1.12
1:A:137:LEU:HD23	1:A:140:ILE:HD11	1.42	1.02
1:F:189:VAL:HG23	1:F:190:VAL:HG23	1.40	1.01
2:B:165:ARG:HH11	2:B:165:ARG:HB3	1.26	1.00
2:B:211:GLU:HG3	4:E:41:VAL:HG21	1.43	1.00
2:G:255:ILE:HG21	3:H:26:TYR:O	1.65	0.97
2:G:7:ASN:HD22	2:G:10:LYS:HB2	1.30	0.96
2:B:118:LEU:H	2:B:118:LEU:CD1	1.77	0.94
2:G:16:ARG:HB3	2:G:16:ARG:NH1	1.83	0.93
4:J:32:SER:OG	4:J:33:PRO:HD3	1.67	0.93
2:B:251:ARG:HH22	2:G:251:ARG:NH2	1.66	0.92
2:B:211:GLU:HG3	4:E:41:VAL:CG2	2.01	0.91
2:B:118:LEU:HD12	2:B:118:LEU:N	1.86	0.90
1:A:127:LYS:HG2	1:A:321:PRO:HG3	1.52	0.89
2:B:16:ARG:HH11	2:B:16:ARG:HB3	1.35	0.89
2:B:251:ARG:HH22	2:G:251:ARG:HH21	0.92	0.88
2:G:23:PRO:HA	2:G:26:ARG:HH12	1.38	0.88
1:A:96:LYS:HG2	1:A:97:GLY:H	1.37	0.87
2:B:17:GLU:O	2:B:20:GLU:HB3	1.73	0.86
1:F:37:ARG:NH1	1:F:42:GLY:HA2	1.91	0.86
1:F:37:ARG:HH12	1:F:42:GLY:HA2	1.39	0.85
1:A:324:LEU:HB3	1:A:327:MET:HE3	1.59	0.84
4:E:60:ASP:HA	4:E:63:LYS:HE2	1.59	0.84
2:G:113:HIS:HB3	2:G:116:GLU:HG3	1.60	0.84
1:F:127:LYS:HG2	1:F:314:PHE:CZ	2.12	0.84
2:B:38:ARG:HA	2:B:66:MET:HE1	1.60	0.83
2:B:70:TYR:OH	2:B:83:VAL:HG21	1.77	0.83
2:G:118:LEU:HD12	2:G:118:LEU:H	1.43	0.83
2:B:86:ALA:HA	2:B:133:LEU:HD21	1.60	0.83
2:B:15:THR:OG1	2:B:18:GLN:HG3	1.78	0.83
2:B:251:ARG:NH2	2:G:251:ARG:HH21	1.76	0.82
1:F:154:ASN:ND2	1:F:167:ASP:HB3	1.95	0.82
1:F:83:GLU:O	1:F:102:VAL:HG23	1.80	0.81
2:B:44:LEU:HG	2:B:48:MET:HE2	1.63	0.80
2:G:23:PRO:HA	2:G:26:ARG:NH1	1.96	0.80
2:G:17:GLU:O	2:G:20:GLU:HB3	1.82	0.79
1:F:94:ARG:HD3	2:G:139:ILE:HD11	1.65	0.79
2:G:256:TRP:HZ3	4:J:54:SER:O	1.66	0.78
2:B:44:LEU:HG	2:B:48:MET:CE	2.14	0.78
2:G:165:ARG:HH11	2:G:165:ARG:HB3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:ASP:HB3	8:G:408:HOH:O	1.83	0.77
2:G:95:GLU:OE1	2:G:95:GLU:HA	1.83	0.76
1:A:22:LEU:HD21	1:A:37:ARG:HG2	1.65	0.76
1:A:295:LEU:HD23	1:A:304:ILE:CG2	2.17	0.75
2:G:165:ARG:HB3	2:G:165:ARG:NH1	2.00	0.75
1:A:10:CYS:SG	1:A:13:CYS:HB3	2.27	0.75
2:G:153:PRO:O	2:G:157:VAL:HG23	1.87	0.75
1:A:193:TRP:HA	1:A:237:GLN:HE22	1.52	0.75
2:B:84:ALA:HB3	2:B:85:PRO:HD3	1.66	0.75
2:G:252:LEU:O	2:G:254:ARG:N	2.21	0.74
2:G:103:HIS:O	2:G:107:VAL:HG23	1.87	0.74
1:F:20:GLU:HB3	1:F:37:ARG:HG3	1.67	0.74
1:A:272:LYS:O	1:A:274:LYS:HG3	1.87	0.74
2:G:84:ALA:HB3	2:G:85:PRO:HD3	1.70	0.74
3:H:25:CYS:HB3	3:H:30:CYS:SG	2.27	0.74
2:G:83:VAL:HG13	2:G:140:ILE:HD11	1.69	0.74
1:F:324:LEU:HD22	1:F:327:MET:HE2	1.69	0.73
1:A:116:ASN:HD22	1:A:119:VAL:HG23	1.53	0.73
2:G:211:GLU:HG3	4:J:41:VAL:CG2	2.19	0.73
2:B:193:PRO:HB2	2:B:194:PRO:HD3	1.70	0.73
2:B:255:ILE:HG21	3:C:26:TYR:O	1.87	0.73
1:F:133:LEU:HD12	1:F:133:LEU:O	1.90	0.72
1:F:146:LEU:HG	1:F:174:PHE:HD1	1.53	0.72
2:B:16:ARG:HH12	2:B:17:GLU:HG2	1.55	0.72
3:H:28:LYS:HB3	4:J:62:MET:SD	2.28	0.72
2:B:258:TRP:HE1	3:H:24:ASN:ND2	1.87	0.72
1:F:94:ARG:O	2:G:135:ILE:HD13	1.89	0.71
1:F:136:GLY:O	1:F:140:ILE:HG23	1.90	0.71
2:G:7:ASN:ND2	2:G:10:LYS:HB2	2.04	0.71
2:G:46:GLN:NE2	2:G:59:ILE:HD13	2.04	0.71
2:B:258:TRP:HD1	2:B:259:ARG:H	1.37	0.71
1:A:295:LEU:HD23	1:A:304:ILE:HG23	1.73	0.70
1:A:262:TYR:C	1:A:264:LYS:H	1.96	0.69
2:G:16:ARG:HH11	2:G:16:ARG:CB	1.96	0.69
1:F:139:TYR:HD1	1:F:142:ARG:NH2	1.90	0.69
2:B:16:ARG:HH11	2:B:16:ARG:CB	2.06	0.69
2:B:101:LEU:HD11	2:B:133:LEU:HD13	1.75	0.69
1:F:175:SER:HB2	3:H:9:GLU:HG3	1.73	0.69
1:A:237:GLN:O	1:A:241:ILE:HG13	1.93	0.69
1:A:20:GLU:HG3	1:A:39:ARG:HH12	1.55	0.69
2:G:52:LEU:CD2	2:G:107:VAL:HG21	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:LYS:O	1:F:145:ILE:HD13	1.94	0.68
1:F:191:THR:HG21	8:F:506:HOH:O	1.93	0.68
2:G:256:TRP:CZ3	4:J:54:SER:O	2.45	0.68
2:G:118:LEU:HD12	2:G:118:LEU:N	2.07	0.68
1:F:67:ILE:O	1:F:71:GLN:HG3	1.94	0.68
1:A:243:GLN:O	1:A:274:LYS:HD2	1.94	0.68
2:G:245:LEU:HB3	4:J:55:MET:HE2	1.74	0.68
2:G:255:ILE:HG21	3:H:27:CYS:HA	1.75	0.68
1:A:123:LEU:HD23	1:A:319:PRO:CG	2.23	0.68
2:G:211:GLU:HG3	4:J:41:VAL:HG21	1.75	0.68
1:A:122:THR:HG23	1:A:125:GLU:OE1	1.92	0.67
2:B:120:ASP:C	2:B:122:ARG:H	1.97	0.67
1:F:244:LEU:HB2	1:F:278:ARG:HH21	1.58	0.67
1:A:99:ILE:HD11	2:B:142:GLN:HE21	1.57	0.67
1:A:262:TYR:C	1:A:262:TYR:HD1	1.98	0.67
2:B:55:SER:HB3	2:B:97:GLN:OE1	1.93	0.67
1:A:37:ARG:NH2	1:A:39:ARG:HA	2.10	0.66
1:A:67:ILE:O	1:A:71:GLN:HG3	1.94	0.66
1:A:73:LEU:HD13	1:A:140:ILE:HG22	1.76	0.66
2:B:258:TRP:HE1	3:H:24:ASN:HD21	1.42	0.66
1:F:122:THR:HG23	1:F:125:GLU:OE1	1.95	0.66
2:G:213:PRO:HG3	4:J:36:ALA:HB3	1.78	0.66
2:B:177:MET:HE2	2:B:203:LEU:HG	1.77	0.66
1:A:262:TYR:O	1:A:264:LYS:N	2.29	0.66
2:B:136:LEU:O	2:B:140:ILE:HG13	1.96	0.65
1:A:15:GLU:HG2	1:A:86:ARG:NH1	2.11	0.65
1:A:96:LYS:CG	1:A:97:GLY:H	2.06	0.65
3:C:1:MET:N	8:C:202:HOH:O	2.26	0.65
1:F:148:ARG:NH1	1:F:172:ARG:CD	2.59	0.65
1:A:31:GLY:HA2	1:A:34:PHE:CZ	2.32	0.65
1:A:262:TYR:C	1:A:262:TYR:CD1	2.71	0.64
2:B:258:TRP:HE1	3:H:24:ASN:CG	1.99	0.64
2:G:136:LEU:O	2:G:140:ILE:HG13	1.98	0.64
1:F:29:THR:OG1	1:F:32:GLU:HB2	1.97	0.64
1:A:116:ASN:HD21	1:A:118:LEU:HB2	1.62	0.63
4:J:44:LYS:HE2	4:J:44:LYS:N	2.13	0.63
2:B:165:ARG:HH11	2:B:165:ARG:CB	2.08	0.63
2:B:17:GLU:CD	2:B:20:GLU:OE2	2.37	0.63
1:A:18:LYS:HG3	1:A:19:TYR:CD2	2.34	0.63
1:A:248:ILE:HG23	1:A:253:TRP:HE3	1.64	0.63
1:A:73:LEU:HD12	1:A:168:PHE:HE1	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:46:GLN:OE1	3:H:35:GLN:HG2	1.97	0.63
1:F:261:LEU:O	1:F:265:LEU:HD23	1.99	0.63
2:B:120:ASP:OD2	2:B:122:ARG:HG3	1.98	0.62
1:F:212:LEU:HD13	1:F:305:ASP:HA	1.79	0.62
1:A:116:ASN:ND2	1:A:119:VAL:HG23	2.14	0.62
1:A:262:TYR:HD1	1:A:262:TYR:O	1.82	0.62
1:A:323:ASP:OD1	1:A:325:LYS:HG3	1.98	0.62
1:A:190:VAL:HG11	1:A:195:ARG:HA	1.81	0.62
2:G:256:TRP:O	3:H:28:LYS:HD3	1.99	0.62
2:G:252:LEU:C	2:G:254:ARG:H	2.03	0.62
1:A:16:VAL:HG11	1:A:87:THR:HG22	1.82	0.62
1:A:107:GLU:HG2	1:A:159:ARG:HB2	1.82	0.62
1:F:290:ASP:OD2	1:F:294:LYS:HE2	2.00	0.62
1:A:49:LYS:HB2	1:A:100:TYR:CE1	2.35	0.61
2:B:195:VAL:O	2:B:199:VAL:HG23	1.99	0.61
2:G:160:CYS:O	2:G:164:VAL:HG22	1.99	0.61
2:B:242:LEU:O	2:B:246:GLU:HG3	2.00	0.61
1:F:75:HIS:HE1	1:F:77:ASN:OD1	1.83	0.61
2:G:47:ASP:O	2:G:51:ARG:HG3	2.00	0.61
2:G:248:THR:C	2:G:250:ASN:H	2.04	0.61
2:B:203:LEU:HD13	2:B:238:THR:HG23	1.83	0.61
2:B:226:ASP:OD1	2:B:228:THR:HG23	1.99	0.61
1:F:189:VAL:HG23	1:F:190:VAL:CG2	2.25	0.61
2:G:203:LEU:HD13	2:G:238:THR:HG23	1.83	0.61
1:A:122:THR:HG23	1:A:125:GLU:CD	2.20	0.61
2:B:158:VAL:HG11	3:C:6:PRO:HD3	1.83	0.61
1:F:31:GLY:HA2	1:F:34:PHE:CZ	2.35	0.61
2:B:252:LEU:O	2:B:254:ARG:N	2.35	0.60
1:F:37:ARG:HH12	1:F:42:GLY:CA	2.12	0.60
3:H:4:VAL:HG11	3:H:13:HIS:ND1	2.15	0.60
1:A:288:ALA:HB2	1:A:314:PHE:HE1	1.66	0.60
1:F:198:GLU:OE2	1:F:300:PRO:HB3	2.01	0.60
1:A:10:CYS:HB3	1:A:86:ARG:HH21	1.65	0.60
1:A:137:LEU:O	1:A:140:ILE:HG12	2.02	0.60
1:A:288:ALA:HB2	1:A:314:PHE:CE1	2.36	0.60
2:B:101:LEU:CD1	2:B:133:LEU:HD13	2.32	0.60
1:F:122:THR:OG1	1:F:125:GLU:HG3	2.02	0.60
1:A:243:GLN:HA	1:A:271:GLN:HE21	1.66	0.60
2:G:138:SER:O	2:G:142:GLN:HG3	2.02	0.60
1:A:189:VAL:O	1:A:190:VAL:HB	2.01	0.60
2:B:213:PRO:HG3	4:E:36:ALA:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:26:ARG:HB2	2:G:26:ARG:CZ	2.30	0.59
1:A:36:ALA:O	1:A:44:LYS:HA	2.03	0.59
1:A:129:VAL:HG11	1:A:222:MET:HE1	1.84	0.59
1:A:193:TRP:CD1	1:A:230:GLN:HA	2.38	0.59
1:F:39:ARG:HH11	1:F:39:ARG:HG2	1.67	0.59
1:A:193:TRP:HA	1:A:237:GLN:NE2	2.17	0.59
2:G:9:ASN:N	2:G:9:ASN:HD22	1.98	0.59
2:G:165:ARG:HH11	2:G:165:ARG:CB	2.15	0.59
1:F:195:ARG:HG3	1:F:199:LEU:HD12	1.83	0.58
1:A:20:GLU:HB2	1:A:39:ARG:NH1	2.17	0.58
1:A:37:ARG:HH22	1:A:39:ARG:HA	1.68	0.58
4:J:61:GLU:HB2	4:J:62:MET:HE2	1.85	0.58
1:A:122:THR:OG1	1:A:125:GLU:HG3	2.03	0.58
1:F:294:LYS:O	1:F:304:ILE:HG22	2.02	0.58
2:B:52:LEU:HG	2:B:107:VAL:HG21	1.86	0.58
2:G:46:GLN:HE21	2:G:59:ILE:HD13	1.68	0.58
2:G:158:VAL:HG11	3:H:6:PRO:HD3	1.85	0.58
1:A:208:PRO:HB2	1:A:209:PRO:HD3	1.84	0.58
4:E:41:VAL:HG12	4:E:41:VAL:O	2.02	0.58
2:B:185:THR:HG22	2:B:244:ILE:HD12	1.86	0.58
1:A:54:ASN:ND2	1:A:60:PRO:HG3	2.19	0.58
3:H:27:CYS:O	3:H:28:LYS:C	2.42	0.58
2:G:120:ASP:C	2:G:122:ARG:H	2.06	0.57
2:G:52:LEU:HD21	2:G:107:VAL:HG21	1.86	0.57
2:G:258:TRP:HD1	2:G:259:ARG:H	1.51	0.57
1:F:120:LYS:HB2	1:F:330:THR:HG21	1.87	0.57
1:F:213:TRP:HE3	1:F:303:ARG:HE	1.52	0.57
1:A:294:LYS:O	1:A:304:ILE:HG22	2.03	0.57
1:F:324:LEU:HB3	1:F:327:MET:HE3	1.86	0.57
4:J:43:SER:C	4:J:44:LYS:HE2	2.25	0.57
2:B:178:ALA:HA	2:B:200:CYS:SG	2.45	0.57
2:B:68:ARG:O	2:B:71:MET:HB2	2.04	0.57
1:A:290:ASP:OD2	1:A:312:HIS:NE2	2.37	0.57
1:F:237:GLN:O	1:F:241:ILE:HG13	2.04	0.57
2:G:255:ILE:CG2	3:H:27:CYS:HA	2.35	0.57
1:A:22:LEU:HG	1:A:36:ALA:HA	1.86	0.57
3:C:28:LYS:HB3	4:E:62:MET:SD	2.45	0.57
2:B:14:PHE:HB2	2:B:19:LEU:HD21	1.86	0.56
1:A:239:ALA:O	1:A:243:GLN:HG3	2.06	0.56
2:G:245:LEU:HB3	4:J:55:MET:CE	2.34	0.56
2:G:248:THR:O	2:G:250:ASN:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG11	1:A:222:MET:CE	2.36	0.56
2:G:46:GLN:HE22	2:G:56:GLN:HE22	1.54	0.56
2:G:102:GLU:HG2	2:G:126:TYR:OH	2.05	0.56
2:G:44:LEU:HD13	3:H:47:TYR:CD1	2.41	0.56
1:F:62:THR:HG23	1:F:63:ALA:N	2.20	0.56
1:A:248:ILE:HG23	1:A:253:TRP:CE3	2.40	0.56
1:A:243:GLN:HG2	1:A:271:GLN:HE21	1.71	0.56
2:G:14:PHE:HB3	2:G:18:GLN:HB2	1.88	0.56
2:B:130:VAL:O	2:B:134:VAL:HG23	2.06	0.55
1:A:25:ILE:HB	1:A:33:VAL:HB	1.88	0.55
1:A:53:GLU:C	1:A:55:GLU:H	2.09	0.55
1:A:54:ASN:O	1:A:54:ASN:CG	2.45	0.55
1:F:307:ASP:OD2	1:F:307:ASP:N	2.26	0.55
1:F:80:ASN:HA	8:F:503:HOH:O	2.06	0.55
2:G:58:THR:HA	2:G:95:GLU:HG3	1.89	0.55
2:G:193:PRO:HB2	2:G:194:PRO:HD3	1.88	0.55
2:B:258:TRP:HD1	2:B:259:ARG:N	2.04	0.55
1:F:228:ILE:HG13	1:F:229:MET:HG3	1.88	0.55
1:A:143:ASN:O	1:A:145:ILE:HG12	2.07	0.54
2:B:106:LYS:HE3	2:B:118:LEU:HD21	1.89	0.54
1:F:148:ARG:NH1	1:F:172:ARG:HD3	2.22	0.54
1:A:116:ASN:ND2	1:A:118:LEU:HB2	2.23	0.54
1:F:149:ASP:O	1:F:151:LYS:HG2	2.08	0.54
2:G:48:MET:HE1	2:G:108:ALA:HB2	1.90	0.54
2:G:192:THR:OG1	2:G:195:VAL:HG23	2.06	0.54
1:A:15:GLU:HG2	1:A:86:ARG:HH12	1.72	0.54
2:B:70:TYR:OH	2:B:83:VAL:CG2	2.53	0.54
2:B:251:ARG:NH2	2:G:251:ARG:NH2	2.43	0.54
2:B:14:PHE:N	2:B:14:PHE:CD2	2.76	0.54
2:G:24:SER:O	2:G:29:VAL:HG23	2.08	0.54
2:G:163:LEU:HD11	4:J:34:LEU:HD23	1.90	0.54
1:A:22:LEU:HD21	1:A:37:ARG:CG	2.34	0.54
1:F:323:ASP:OD2	1:F:323:ASP:C	2.46	0.54
2:G:220:HIS:N	2:G:223:GLU:OE1	2.35	0.54
1:A:54:ASN:HD22	1:A:60:PRO:HG3	1.73	0.53
1:F:94:ARG:CD	2:G:139:ILE:HD11	2.37	0.53
2:B:127:LEU:O	2:B:131:GLN:HG2	2.08	0.53
2:G:51:ARG:HB2	2:G:107:VAL:HG11	1.88	0.53
1:A:97:GLY:HA3	8:A:509:HOH:O	2.08	0.53
1:F:185:TYR:HB2	1:F:206:TYR:CE1	2.44	0.53
2:G:46:GLN:NE2	2:G:59:ILE:CD1	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:PRO:O	2:B:83:VAL:HG23	2.08	0.53
2:B:134:VAL:O	2:B:137:GLU:HB3	2.09	0.53
2:G:101:LEU:CD1	2:G:133:LEU:HD23	2.39	0.53
2:B:255:ILE:HG23	3:H:24:ASN:ND2	2.23	0.53
1:F:206:TYR:CD2	1:F:210:ILE:HD13	2.44	0.53
2:G:101:LEU:HD11	2:G:133:LEU:HD23	1.90	0.53
2:G:259:ARG:HG2	2:G:259:ARG:HH21	1.74	0.53
1:A:283:VAL:O	1:A:284:ARG:HB2	2.09	0.53
1:A:329:SER:O	1:A:330:THR:O	2.27	0.53
2:G:120:ASP:O	2:G:122:ARG:N	2.42	0.53
1:A:29:THR:OG1	1:A:32:GLU:HB2	2.09	0.52
1:F:37:ARG:NH1	1:F:37:ARG:HB2	2.24	0.52
1:F:90:SER:HB3	1:F:93:ASN:OD1	2.09	0.52
4:J:32:SER:CB	4:J:33:PRO:HD3	2.37	0.52
2:G:210:TRP:CZ2	4:J:40:LYS:HE3	2.44	0.52
1:A:262:TYR:C	1:A:264:LYS:N	2.62	0.52
2:G:95:GLU:OE1	2:G:95:GLU:CA	2.55	0.52
3:C:8:LEU:HD22	3:C:12:LYS:HB3	1.92	0.52
2:G:57:LEU:HD12	8:G:402:HOH:O	2.09	0.52
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.75	0.52
1:A:312:HIS:ND1	1:A:313:ASP:N	2.57	0.52
2:B:54:VAL:HG12	2:B:99:LYS:HE2	1.92	0.52
1:F:35:LYS:HG3	1:F:105:PHE:CE1	2.44	0.52
3:C:24:ASN:OD1	2:G:258:TRP:NE1	2.42	0.52
1:F:195:ARG:CG	1:F:199:LEU:HD12	2.40	0.52
3:H:27:CYS:O	3:H:29:LYS:N	2.43	0.52
1:A:123:LEU:HD23	1:A:319:PRO:HG3	1.92	0.52
2:B:208:SER:HB3	4:E:59:TYR:CD2	2.45	0.52
1:F:94:ARG:HH11	1:F:94:ARG:CB	2.23	0.52
2:G:163:LEU:O	2:G:163:LEU:HD12	2.10	0.52
1:F:207:GLY:C	1:F:209:PRO:HD2	2.30	0.52
1:F:279:LEU:CD1	1:F:292:ILE:HG21	2.40	0.51
2:G:37:TYR:HB3	2:G:75:PHE:CE1	2.45	0.51
1:A:323:ASP:OD2	1:A:323:ASP:C	2.48	0.51
2:G:192:THR:O	2:G:196:VAL:HG23	2.11	0.51
1:A:77:ASN:HD21	1:A:132:MET:HG2	1.74	0.51
3:C:24:ASN:ND2	2:G:255:ILE:HG23	2.26	0.51
2:G:43:ASN:ND2	3:H:39:ILE:HG21	2.25	0.51
2:G:17:GLU:O	2:G:20:GLU:CB	2.57	0.51
4:J:52:ILE:HD11	4:J:56:LEU:HD11	1.93	0.51
4:J:58:ASN:HB3	4:J:61:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD12	1:A:168:PHE:CE1	2.46	0.51
2:B:25:ARG:HH12	2:B:31:PRO:N	2.09	0.51
2:G:39:GLN:HB3	3:H:45:ILE:HD13	1.92	0.51
2:B:184:LEU:O	2:B:244:ILE:HG21	2.11	0.50
4:J:41:VAL:O	4:J:44:LYS:HE3	2.11	0.50
1:A:89:ALA:HB2	1:A:97:GLY:CA	2.41	0.50
1:F:214:GLY:O	1:F:218:ILE:HG13	2.11	0.50
2:G:7:ASN:ND2	2:G:10:LYS:CB	2.73	0.50
2:G:54:VAL:HG12	2:G:99:LYS:HE2	1.93	0.50
1:A:89:ALA:HB2	1:A:97:GLY:HA2	1.94	0.50
2:B:120:ASP:C	2:B:122:ARG:N	2.65	0.50
1:F:39:ARG:HG2	1:F:39:ARG:NH1	2.26	0.50
2:G:44:LEU:HD13	3:H:47:TYR:CE1	2.46	0.50
2:B:256:TRP:CH2	4:E:57:GLY:HA2	2.47	0.50
1:F:263:GLU:O	1:F:264:LYS:C	2.49	0.50
1:F:283:VAL:O	1:F:284:ARG:HB2	2.12	0.50
1:A:31:GLY:HA2	1:A:34:PHE:CE2	2.46	0.50
1:A:67:ILE:HG23	1:A:84:ILE:HD11	1.92	0.50
2:B:205:CYS:HB3	2:B:210:TRP:O	2.12	0.50
1:F:117:VAL:HG12	1:F:117:VAL:O	2.10	0.50
1:A:16:VAL:CG1	1:A:87:THR:HG22	2.40	0.50
1:A:326:GLY:O	1:A:329:SER:HB2	2.12	0.50
1:F:56:LYS:O	2:G:101:LEU:HD22	2.12	0.50
2:G:184:LEU:N	2:G:184:LEU:HD23	2.25	0.50
1:A:256:VAL:HG13	1:A:262:TYR:CE2	2.46	0.50
2:B:153:PRO:O	2:B:157:VAL:HG23	2.11	0.50
2:G:7:ASN:HD22	2:G:10:LYS:CB	2.13	0.50
3:H:29:LYS:HG2	4:J:65:PHE:CE1	2.47	0.50
2:B:14:PHE:HB3	2:B:18:GLN:HB2	1.94	0.50
1:A:10:CYS:N	1:A:11:PRO:CD	2.75	0.50
1:A:218:ILE:O	1:A:221:GLU:HB2	2.11	0.50
1:F:88:LYS:HA	8:F:517:HOH:O	2.12	0.50
2:G:60:ASN:ND2	2:G:154:HIS:CE1	2.80	0.50
1:A:132:MET:HB3	1:A:163:LEU:HB3	1.92	0.49
1:A:116:ASN:HD22	1:A:119:VAL:CG2	2.23	0.49
1:A:139:TYR:O	1:A:143:ASN:ND2	2.37	0.49
2:B:17:GLU:HA	2:B:20:GLU:OE2	2.12	0.49
1:A:96:LYS:CG	1:A:97:GLY:N	2.74	0.49
2:B:120:ASP:O	2:B:122:ARG:N	2.45	0.49
1:A:61:ILE:HG23	1:A:62:THR:N	2.27	0.49
1:A:219:MET:CE	1:A:292:ILE:HG13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:52:LEU:O	2:G:99:LYS:HE3	2.13	0.49
1:F:8:VAL:HG22	1:F:91:PRO:HD3	1.94	0.49
1:F:196:PRO:HB2	1:F:198:GLU:OE1	2.13	0.49
1:A:75:HIS:CD2	1:A:77:ASN:H	2.31	0.49
3:H:1:MET:HE3	4:J:66:ILE:HG23	1.95	0.49
1:A:99:ILE:HD11	2:B:142:GLN:NE2	2.27	0.48
2:G:260:ALA:HB1	3:H:29:LYS:NZ	2.28	0.48
1:F:25:ILE:HD11	1:F:105:PHE:HE1	1.77	0.48
1:A:73:LEU:CD1	1:A:168:PHE:HE1	2.26	0.48
1:F:75:HIS:ND1	1:F:76:GLU:N	2.61	0.48
3:H:5:ASP:OD2	3:H:7:ARG:HB2	2.13	0.48
2:B:24:SER:HA	2:B:74:SER:OG	2.14	0.48
1:A:121:PHE:CZ	1:A:327:MET:HG3	2.48	0.48
1:A:237:GLN:HG3	1:A:241:ILE:HD11	1.96	0.48
1:F:254:PRO:O	1:F:255:ASN:HB2	2.12	0.48
2:G:7:ASN:O	2:G:11:ARG:N	2.46	0.48
3:H:36:VAL:O	3:H:40:THR:HG23	2.14	0.48
1:A:144:LYS:HA	1:A:174:PHE:CE1	2.48	0.48
2:B:7:ASN:O	2:B:11:ARG:N	2.46	0.48
1:F:116:ASN:ND2	1:F:119:VAL:HG23	2.28	0.48
2:G:97:GLN:N	2:G:98:PRO:CD	2.77	0.48
1:F:247:SER:OG	1:F:271:GLN:HB2	2.14	0.48
2:G:9:ASN:N	2:G:9:ASN:ND2	2.61	0.48
2:B:126:TYR:CD2	2:B:127:LEU:HD23	2.49	0.48
2:B:254:ARG:HG2	2:G:114:PRO:HG2	1.96	0.48
1:F:127:LYS:NZ	1:F:317:SER:O	2.47	0.48
1:F:197:PRO:HG3	1:F:241:ILE:HG21	1.95	0.48
1:F:243:GLN:HA	1:F:271:GLN:HE21	1.79	0.48
2:G:7:ASN:HA	2:G:10:LYS:HB2	1.96	0.48
2:B:158:VAL:HG11	3:C:6:PRO:CD	2.43	0.47
3:H:1:MET:CE	4:J:66:ILE:HG23	2.44	0.47
1:A:123:LEU:HD23	1:A:319:PRO:CD	2.43	0.47
1:A:159:ARG:HA	8:A:507:HOH:O	2.13	0.47
1:A:324:LEU:HB3	1:A:327:MET:CE	2.36	0.47
2:B:250:ASN:O	2:B:250:ASN:ND2	2.42	0.47
4:E:46:ASP:OD1	4:E:46:ASP:C	2.52	0.47
4:E:52:ILE:HD11	4:E:56:LEU:HD12	1.95	0.47
1:A:256:VAL:HG13	1:A:262:TYR:HE2	1.79	0.47
1:A:299:ASP:OD2	1:A:301:ALA:HB3	2.13	0.47
1:F:133:LEU:HD13	1:F:165:LEU:HD21	1.96	0.47
2:G:25:ARG:CZ	2:G:31:PRO:HG3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:66:MET:SD	2:G:67:HIS:N	2.88	0.47
2:B:105:ILE:HG21	2:B:126:TYR:CE1	2.49	0.47
2:B:214:VAL:HG12	2:B:215:SER:N	2.29	0.47
2:G:256:TRP:CD1	2:G:256:TRP:C	2.87	0.47
2:B:248:THR:C	2:B:250:ASN:H	2.18	0.47
2:B:44:LEU:HG	2:B:48:MET:HE1	1.96	0.47
1:F:107:GLU:OE2	1:F:159:ARG:HD3	2.14	0.47
1:A:203:GLU:OE2	1:A:205:ASP:HB3	2.15	0.47
2:G:185:THR:HG22	2:G:244:ILE:HD12	1.96	0.47
1:F:32:GLU:OE1	1:F:33:VAL:HG23	2.15	0.47
1:F:77:ASN:O	1:F:164:LYS:HA	2.14	0.47
2:G:83:VAL:O	2:G:84:ALA:C	2.53	0.47
1:A:37:ARG:HA	1:A:43:GLN:O	2.15	0.47
1:A:122:THR:N	1:A:125:GLU:OE1	2.44	0.47
1:A:123:LEU:HD21	1:A:285:ASP:OD2	2.15	0.47
1:A:127:LYS:HE2	1:A:314:PHE:CE2	2.50	0.47
2:G:155:THR:HG22	2:G:156:HIS:N	2.30	0.47
1:A:22:LEU:HD11	1:A:37:ARG:HB3	1.97	0.46
2:B:86:ALA:HA	2:B:133:LEU:CD2	2.36	0.46
1:F:72:LEU:HD23	1:F:73:LEU:HD23	1.96	0.46
1:A:187:ASN:HB2	1:A:204:ARG:HG2	1.96	0.46
1:A:261:LEU:O	1:A:264:LYS:HB3	2.15	0.46
2:B:182:LEU:HD23	8:B:411:HOH:O	2.13	0.46
2:B:220:HIS:HB2	2:B:223:GLU:HG3	1.98	0.46
1:F:144:LYS:HA	1:F:174:PHE:CZ	2.51	0.46
2:G:60:ASN:HD21	2:G:154:HIS:CE1	2.32	0.46
2:G:118:LEU:H	2:G:118:LEU:CD1	2.10	0.46
2:B:160:CYS:O	2:B:164:VAL:HG22	2.14	0.46
1:F:22:LEU:HD21	1:F:37:ARG:HG2	1.97	0.46
1:F:191:THR:CG2	8:F:512:HOH:O	2.63	0.46
1:F:208:PRO:N	1:F:209:PRO:CD	2.78	0.46
1:A:151:LYS:HG2	1:A:154:ASN:HD22	1.80	0.46
2:B:17:GLU:O	2:B:20:GLU:CB	2.55	0.46
1:F:37:ARG:HA	1:F:43:GLN:O	2.15	0.46
2:G:82:SER:O	2:G:136:LEU:HD12	2.15	0.46
2:B:252:LEU:C	2:B:254:ARG:H	2.19	0.46
1:F:273:ARG:CZ	1:F:275:VAL:HG21	2.45	0.46
2:G:178:ALA:HA	2:G:200:CYS:SG	2.56	0.46
2:G:233:LEU:HD12	2:G:233:LEU:O	2.16	0.46
1:A:73:LEU:HD22	1:A:139:TYR:CE2	2.51	0.46
1:F:181:GLN:HA	1:F:182:PRO:HD3	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:56:GLN:HE21	2:G:59:ILE:HB	1.81	0.46
2:G:236:GLU:O	2:G:239:HIS:HB3	2.15	0.46
2:B:27:PHE:N	2:B:27:PHE:CD2	2.84	0.46
2:B:95:GLU:OE1	2:B:95:GLU:HA	2.15	0.46
2:B:173:THR:O	2:B:176:PHE:HB3	2.16	0.46
2:B:222:TRP:CH2	2:B:231:LEU:HD13	2.51	0.46
3:H:4:VAL:HG11	3:H:13:HIS:CE1	2.51	0.46
1:A:18:LYS:HG3	1:A:19:TYR:CE2	2.50	0.46
1:A:137:LEU:CD2	1:A:140:ILE:HD11	2.31	0.46
4:E:60:ASP:HA	4:E:63:LYS:CE	2.37	0.46
2:B:210:TRP:CZ3	4:E:40:LYS:HG2	2.51	0.46
1:A:232:ASN:N	1:A:236:HIS:ND1	2.61	0.45
1:A:279:LEU:CD1	1:A:292:ILE:HG21	2.46	0.45
2:G:44:LEU:HD23	2:G:84:ALA:HB3	1.98	0.45
2:B:7:ASN:HA	2:B:10:LYS:HB2	1.99	0.45
2:B:126:TYR:HD2	2:B:127:LEU:HD23	1.81	0.45
1:F:297:VAL:HB	1:F:303:ARG:HA	1.98	0.45
2:B:34:GLU:HA	2:B:37:TYR:HD2	1.81	0.45
1:F:148:ARG:NH1	1:F:172:ARG:HD2	2.32	0.45
1:F:236:HIS:O	1:F:239:ALA:HB3	2.16	0.45
2:G:82:SER:OG	2:G:136:LEU:HD11	2.17	0.45
1:A:159:ARG:HB3	1:A:159:ARG:HH11	1.81	0.45
1:A:192:LEU:HG	1:A:237:GLN:NE2	2.32	0.45
2:B:84:ALA:HB3	2:B:85:PRO:CD	2.43	0.45
2:G:63:ILE:HD13	2:G:183:HIS:HD2	1.82	0.45
2:G:252:LEU:CB	8:G:405:HOH:O	2.64	0.45
2:G:255:ILE:O	2:G:255:ILE:HG22	2.16	0.45
2:B:120:ASP:CG	2:B:122:ARG:HG3	2.37	0.45
2:B:163:LEU:HD21	4:E:35:PHE:CE2	2.52	0.45
1:F:62:THR:CG2	1:F:63:ALA:N	2.80	0.45
1:A:219:MET:HG2	1:A:292:ILE:HD11	1.98	0.45
1:F:253:TRP:CG	1:F:256:VAL:HB	2.52	0.45
1:A:151:LYS:HE2	1:A:154:ASN:HD21	1.82	0.45
1:F:96:LYS:HG3	2:G:138:SER:OG	2.17	0.45
1:F:127:LYS:HE2	1:F:314:PHE:CE1	2.51	0.45
1:F:276:LYS:CG	1:F:289:LEU:HB3	2.47	0.45
3:H:5:ASP:HA	3:H:6:PRO:HD3	1.79	0.45
1:A:142:ARG:NH1	1:A:142:ARG:HG3	2.33	0.44
2:B:14:PHE:HB2	2:B:19:LEU:CD2	2.47	0.44
2:B:123:SER:O	2:B:127:LEU:HG	2.16	0.44
1:F:80:ASN:ND2	1:F:104:ASP:OD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:CE1	1:A:327:MET:HG3	2.52	0.44
1:A:236:HIS:O	1:A:240:LEU:HG	2.17	0.44
1:F:87:THR:HB	1:F:88:LYS:HE3	1.99	0.44
2:B:27:PHE:N	2:B:27:PHE:HD2	2.14	0.44
1:F:236:HIS:O	1:F:236:HIS:HD2	1.99	0.44
1:A:196:PRO:HG2	1:A:199:LEU:HG	1.99	0.44
1:A:243:GLN:HA	1:A:271:GLN:NE2	2.31	0.44
1:A:224:THR:O	1:A:225:ARG:HB2	2.18	0.44
1:F:117:VAL:HA	1:F:225:ARG:HH12	1.83	0.44
1:F:253:TRP:HA	1:F:299:ASP:HB2	2.00	0.44
1:F:189:VAL:CG2	1:F:190:VAL:HG23	2.28	0.44
1:A:54:ASN:HD22	1:A:60:PRO:CG	2.30	0.44
2:B:103:HIS:O	2:B:107:VAL:HG23	2.18	0.44
2:B:258:TRP:CD1	2:B:259:ARG:N	2.84	0.44
1:F:244:LEU:HB2	1:F:278:ARG:NH2	2.30	0.44
1:F:285:ASP:HA	1:F:286:PRO:HD3	1.87	0.44
2:B:135:ILE:O	2:B:139:ILE:HG13	2.19	0.43
1:F:9:GLU:HG3	1:F:11:PRO:HD3	2.00	0.43
1:F:20:GLU:HB3	1:F:37:ARG:CG	2.44	0.43
2:G:202:HIS:HB2	2:G:234:LEU:HD13	2.00	0.43
2:B:55:SER:OG	2:B:57:LEU:HB3	2.18	0.43
2:G:24:SER:HB2	2:G:34:GLU:OE1	2.17	0.43
2:G:184:LEU:HD11	3:H:43:LEU:CD1	2.48	0.43
2:G:56:GLN:NE2	2:G:59:ILE:HB	2.32	0.43
1:A:192:LEU:HD11	1:A:237:GLN:HB2	2.00	0.43
1:F:236:HIS:CD2	1:F:236:HIS:C	2.92	0.43
2:G:109:HIS:CE1	2:G:113:HIS:HB2	2.53	0.43
2:B:59:ILE:O	2:B:63:ILE:HG13	2.18	0.43
2:B:105:ILE:HG21	2:B:126:TYR:HE1	1.84	0.43
2:B:176:PHE:CE1	3:C:1:MET:CE	3.02	0.43
3:C:37:CYS:O	3:C:41:LYS:HB2	2.18	0.43
1:A:243:GLN:HG2	1:A:271:GLN:NE2	2.32	0.43
6:B:304:SO4:O3	4:E:63:LYS:HD2	2.19	0.43
1:F:146:LEU:CD2	1:F:174:PHE:CD1	3.01	0.43
2:G:68:ARG:NH2	8:G:401:HOH:O	2.48	0.43
2:B:58:THR:HA	2:B:95:GLU:HG3	2.00	0.43
2:G:192:THR:HB	2:G:194:PRO:HD2	2.00	0.43
1:A:87:THR:O	1:A:88:LYS:C	2.56	0.43
1:F:25:ILE:HB	1:F:33:VAL:HG12	2.00	0.43
2:G:15:THR:HG23	2:G:18:GLN:OE1	2.18	0.43
2:G:44:LEU:O	2:G:48:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:250:ASN:ND2	8:G:405:HOH:O	2.52	0.43
2:G:252:LEU:C	2:G:254:ARG:N	2.65	0.43
1:A:137:LEU:HA	1:A:140:ILE:CD1	2.49	0.43
2:B:23:PRO:O	2:B:26:ARG:HB2	2.19	0.43
1:F:123:LEU:HD23	1:F:319:PRO:CG	2.49	0.43
1:A:212:LEU:HD13	1:A:305:ASP:HA	2.01	0.42
1:F:239:ALA:O	1:F:243:GLN:HG3	2.19	0.42
1:F:276:LYS:HG2	1:F:289:LEU:HB3	2.01	0.42
1:A:17:SER:O	1:A:19:TYR:N	2.52	0.42
2:B:258:TRP:NE1	3:H:24:ASN:OD1	2.47	0.42
1:A:107:GLU:CD	1:A:107:GLU:H	2.23	0.42
2:B:236:GLU:O	2:B:239:HIS:HB3	2.20	0.42
3:C:31:CYS:O	3:C:38:PHE:HA	2.18	0.42
1:F:16:VAL:HG23	1:F:86:ARG:O	2.19	0.42
1:F:154:ASN:ND2	1:F:167:ASP:CB	2.77	0.42
3:H:8:LEU:CD2	3:H:12:LYS:HB3	2.49	0.42
1:A:109:ASP:O	1:A:109:ASP:OD2	2.37	0.42
1:A:127:LYS:HE2	1:A:314:PHE:CZ	2.54	0.42
1:A:267:LEU:HD12	8:A:520:HOH:O	2.20	0.42
1:F:16:VAL:HG12	1:F:16:VAL:O	2.19	0.42
1:A:32:GLU:HG2	1:A:33:VAL:HG22	2.00	0.42
2:B:83:VAL:HA	2:B:136:LEU:CD2	2.49	0.42
2:G:181:SER:HA	2:G:241:PHE:HE1	1.84	0.42
1:A:37:ARG:CZ	1:A:39:ARG:HA	2.49	0.42
1:A:283:VAL:O	1:A:284:ARG:CB	2.68	0.42
2:B:8:ASN:HD22	2:B:8:ASN:HA	1.74	0.42
4:J:44:LYS:HE2	4:J:44:LYS:CA	2.50	0.42
3:C:40:THR:O	3:C:44:GLY:HA2	2.18	0.42
1:F:80:ASN:HB3	1:F:104:ASP:OD2	2.19	0.42
1:F:216:GLY:HA2	1:F:295:LEU:HD13	2.02	0.42
1:F:268:VAL:CG2	1:F:271:GLN:HG2	2.50	0.42
2:G:16:ARG:NH1	2:G:16:ARG:CB	2.68	0.42
2:G:248:THR:C	2:G:250:ASN:N	2.73	0.42
1:A:159:ARG:HG3	8:A:507:HOH:O	2.20	0.42
1:A:198:GLU:HG2	1:A:199:LEU:H	1.85	0.42
1:A:221:GLU:HA	1:A:224:THR:OG1	2.20	0.42
1:A:329:SER:O	1:A:330:THR:C	2.58	0.42
2:B:252:LEU:C	2:B:254:ARG:N	2.73	0.42
1:F:127:LYS:HG2	1:F:314:PHE:CE2	2.53	0.42
1:F:146:LEU:HG	1:F:174:PHE:CD1	2.43	0.42
1:A:248:ILE:HG12	1:A:298:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:HB2	4:E:51:ARG:NH2	2.35	0.42
1:F:267:LEU:O	1:F:268:VAL:C	2.57	0.42
2:G:240:GLU:O	2:G:244:ILE:HG13	2.18	0.42
1:A:122:THR:O	1:A:125:GLU:N	2.52	0.42
2:B:167:SER:OG	6:B:304:SO4:O2	2.27	0.42
1:F:8:VAL:HG22	1:F:91:PRO:HG3	2.02	0.42
1:F:156:LEU:HD12	1:F:166:ALA:HB2	2.01	0.42
1:A:127:LYS:HE3	1:A:127:LYS:HB2	1.89	0.41
1:A:219:MET:HG2	1:A:292:ILE:CG1	2.50	0.41
2:G:260:ALA:HB1	3:H:29:LYS:HZ2	1.84	0.41
4:J:63:LYS:HE2	4:J:63:LYS:HB3	1.85	0.41
1:A:28:GLY:HA3	1:A:32:GLU:OE1	2.20	0.41
1:A:181:GLN:HA	1:A:182:PRO:HD3	1.86	0.41
1:A:198:GLU:HG2	1:A:199:LEU:N	2.35	0.41
1:A:253:TRP:HB3	1:A:256:VAL:HB	2.02	0.41
1:A:299:ASP:HA	1:A:300:PRO:HD2	1.93	0.41
1:F:128:ARG:HA	1:F:128:ARG:HD2	1.84	0.41
1:F:148:ARG:HH12	1:F:172:ARG:HD2	1.85	0.41
1:F:244:LEU:HD13	1:F:278:ARG:HE	1.85	0.41
2:G:52:LEU:HD21	2:G:107:VAL:CG2	2.48	0.41
2:G:101:LEU:CD2	2:G:130:VAL:HG13	2.50	0.41
2:G:140:ILE:O	2:G:144:LEU:HG	2.20	0.41
2:G:245:LEU:O	4:J:55:MET:HE1	2.19	0.41
1:A:17:SER:C	1:A:19:TYR:N	2.73	0.41
1:A:82:ILE:HB	1:A:102:VAL:O	2.20	0.41
2:B:165:ARG:HB3	2:B:165:ARG:NH1	2.10	0.41
4:E:52:ILE:HD11	4:E:56:LEU:CD1	2.51	0.41
2:G:63:ILE:HG21	2:G:182:LEU:O	2.20	0.41
2:G:106:LYS:NZ	2:G:118:LEU:HD21	2.34	0.41
3:H:5:ASP:O	3:H:8:LEU:HB2	2.20	0.41
2:G:120:ASP:C	2:G:122:ARG:N	2.73	0.41
2:G:120:ASP:OD2	2:G:122:ARG:HB2	2.20	0.41
4:J:58:ASN:CG	4:J:61:GLU:HG3	2.40	0.41
1:A:253:TRP:CG	1:A:256:VAL:HB	2.56	0.41
1:A:320:MET:HB3	1:A:321:PRO:CD	2.51	0.41
3:C:25:CYS:SG	3:C:26:TYR:N	2.93	0.41
1:F:148:ARG:HH12	1:F:172:ARG:CD	2.32	0.41
2:G:116:GLU:H	2:G:116:GLU:HG2	1.53	0.41
2:G:233:LEU:HD12	2:G:237:LEU:HG	2.03	0.41
1:A:17:SER:C	1:A:19:TYR:H	2.23	0.41
1:A:188:ARG:O	1:A:189:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LYS:HE3	2:B:159:LYS:HB2	1.87	0.41
2:G:195:VAL:O	2:G:199:VAL:HG23	2.20	0.41
3:H:19:LYS:HA	3:H:19:LYS:HD3	1.80	0.41
1:A:53:GLU:C	1:A:55:GLU:N	2.73	0.41
2:B:90:LEU:O	2:B:93:LYS:N	2.52	0.41
2:B:251:ARG:HD2	3:C:41:LYS:O	2.21	0.41
2:G:63:ILE:CD1	2:G:183:HIS:CD2	3.04	0.41
2:B:97:GLN:N	2:B:98:PRO:CD	2.83	0.41
2:B:242:LEU:CB	4:E:51:ARG:NH2	2.84	0.41
3:H:5:ASP:HB3	3:H:8:LEU:HD12	2.01	0.41
1:A:119:VAL:O	1:A:225:ARG:NH2	2.52	0.41
2:B:121:THR:HA	2:B:126:TYR:CD2	2.56	0.41
3:C:27:CYS:O	3:C:28:LYS:C	2.60	0.41
1:F:175:SER:CB	3:H:9:GLU:HG3	2.46	0.41
2:G:58:THR:HG21	2:G:92:ALA:HA	2.02	0.41
2:G:217:ASP:N	2:G:217:ASP:OD2	2.54	0.41
1:A:19:TYR:CD1	1:A:45:VAL:HG21	2.56	0.41
1:A:273:ARG:HH11	1:A:273:ARG:HG3	1.86	0.41
2:B:208:SER:HB3	4:E:59:TYR:CE2	2.56	0.41
2:G:101:LEU:HD21	2:G:130:VAL:HG13	2.02	0.41
1:A:137:LEU:HA	1:A:140:ILE:HD11	2.03	0.40
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.86	0.40
1:A:279:LEU:O	1:A:283:VAL:HG23	2.20	0.40
1:F:68:LYS:CE	2:G:94:VAL:HG13	2.51	0.40
1:F:193:TRP:CD1	1:F:193:TRP:N	2.87	0.40
1:F:255:ASN:C	1:F:257:ASP:H	2.23	0.40
1:F:256:VAL:O	1:F:256:VAL:HG22	2.21	0.40
1:F:272:LYS:O	1:F:274:LYS:CG	2.70	0.40
2:B:83:VAL:HA	2:B:136:LEU:HD22	2.04	0.40
2:B:167:SER:OG	2:B:168:LYS:N	2.54	0.40
1:F:143:ASN:O	1:F:145:ILE:HG12	2.21	0.40
2:B:16:ARG:HH11	2:B:16:ARG:CG	2.34	0.40
1:F:47:LEU:HD23	1:F:102:VAL:HG13	2.04	0.40
2:G:65:TYR:O	2:G:69:PHE:HB2	2.22	0.40

All (8) 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:A:263:GLU:OE2	5:E:101:YT3:Y[2_556]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:GLU:OE2	5:B:303:YT3:Y[2_555]	1.70	0.50
2:G:17:GLU:OE2	5:G:301:YT3:Y[2_555]	1.80	0.40
5:A:403:YT3:Y	5:B:302:YT3:Y[2_556]	1.95	0.25
2:B:124:GLU:OE1	5:F:403:YT3:Y[2_555]	1.95	0.25
2:B:20:GLU:OE1	5:B:303:YT3:Y[2_555]	2.02	0.18
1:A:311:ASN:OD1	5:F:401:YT3:Y[3_445]	2.03	0.17
1:A:266:GLU:OE1	5:E:101:YT3:Y[2_556]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/326 (97%)	267 (85%)	35 (11%)	13 (4%)	3	11
1	F	322/326 (99%)	273 (85%)	39 (12%)	10 (3%)	4	16
2	B	254/266 (96%)	228 (90%)	22 (9%)	4 (2%)	9	32
2	G	253/266 (95%)	225 (89%)	22 (9%)	6 (2%)	6	22
3	C	46/48 (96%)	41 (89%)	5 (11%)	0	100	100
3	H	46/48 (96%)	40 (87%)	5 (11%)	1 (2%)	6	24
4	E	36/43 (84%)	32 (89%)	3 (8%)	1 (3%)	5	19
4	J	36/43 (84%)	29 (81%)	6 (17%)	1 (3%)	5	19
All	All	1308/1366 (96%)	1135 (87%)	137 (10%)	36 (3%)	5	19

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	263	GLU
1	A	330	THR
2	B	121	THR
2	B	253	LYS

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Mol	Chain	Res	Type
4	E	63	LYS
2	G	116	GLU
2	G	253	LYS
2	G	256	TRP
3	H	28	LYS
1	A	180	SER
2	B	116	GLU
1	F	190	VAL
1	F	264	LYS
2	G	121	THR
1	A	55	GLU
1	A	190	VAL
1	A	266	GLU
1	A	323	ASP
2	B	250	ASN
1	F	89	ALA
1	F	167	ASP
2	G	250	ASN
1	A	56	LYS
1	F	94	ARG
4	J	45	GLU
1	A	18	LYS
1	A	275	VAL
1	A	329	SER
1	F	90	SER
1	F	298	LEU
2	G	249	PRO
1	F	275	VAL
1	F	91	PRO
1	F	97	GLY
1	A	209	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/288 (98%)	268 (95%)	14 (5%)	24	57
1	F	287/288 (100%)	273 (95%)	14 (5%)	25	57
2	B	234/241 (97%)	216 (92%)	18 (8%)	13	35
2	G	233/241 (97%)	216 (93%)	17 (7%)	14	38
3	C	43/43 (100%)	42 (98%)	1 (2%)	50	80
3	H	43/43 (100%)	40 (93%)	3 (7%)	15	41
4	E	35/38 (92%)	32 (91%)	3 (9%)	10	30
4	J	35/38 (92%)	33 (94%)	2 (6%)	20	51
All	All	1192/1220 (98%)	1120 (94%)	72 (6%)	19	49

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	55	GLU
1	A	128	ARG
1	A	130	MET
1	A	133	LEU
1	A	159	ARG
1	A	181	GLN
1	A	208	PRO
1	A	212	LEU
1	A	255	ASN
1	A	262	TYR
1	A	267	LEU
1	A	307	ASP
1	A	331	HIS
2	B	8	ASN
2	B	9	ASN
2	B	16	ARG
2	B	27	PHE
2	B	30	ASP
2	B	66	MET
2	B	118	LEU
2	B	121	THR
2	B	133	LEU
2	B	136	LEU

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Mol	Chain	Res	Type
2	B	165	ARG
2	B	186	THR
2	B	194	PRO
2	B	228	THR
2	B	241	PHE
2	B	250	ASN
2	B	256	TRP
2	B	258	TRP
3	C	20	THR
4	E	44	LYS
4	E	50	SER
4	E	54	SER
1	F	14	ASP
1	F	37	ARG
1	F	79	VAL
1	F	94	ARG
1	F	102	VAL
1	F	108	HIS
1	F	135	ASN
1	F	140	ILE
1	F	179	ASN
1	F	189	VAL
1	F	209	PRO
1	F	255	ASN
1	F	257	ASP
1	F	307	ASP
2	G	7	ASN
2	G	9	ASN
2	G	16	ARG
2	G	31	PRO
2	G	72	ILE
2	G	95	GLU
2	G	116	GLU
2	G	118	LEU
2	G	165	ARG
2	G	168	LYS
2	G	179	THR
2	G	181	SER
2	G	230	THR
2	G	252	LEU
2	G	256	TRP
2	G	258	TRP

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Mol	Chain	Res	Type
2	G	261	CYS
3	H	2	GLU
3	H	8	LEU
3	H	20	THR
4	J	44	LYS
4	J	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	75	HIS
1	A	77	ASN
1	A	116	ASN
1	A	154	ASN
1	A	187	ASN
1	A	232	ASN
1	A	237	GLN
1	A	243	GLN
1	A	255	ASN
1	A	271	GLN
2	B	7	ASN
2	B	8	ASN
2	B	50	GLN
2	B	128	GLN
2	B	131	GLN
2	B	142	GLN
2	B	162	GLN
2	B	190	GLN
3	C	24	ASN
1	F	143	ASN
1	F	154	ASN
1	F	232	ASN
1	F	236	HIS
1	F	243	GLN
1	F	255	ASN
2	G	7	ASN
2	G	8	ASN
2	G	9	ASN
2	G	46	GLN
2	G	50	GLN
2	G	56	GLN

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Mol	Chain	Res	Type
2	G	60	ASN
2	G	77	GLN
2	G	129	GLN
2	G	142	GLN
2	G	190	GLN
2	G	202	HIS
2	G	250	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	A	186	1	8,10,11	1.46	1 (12%)	10,14,16	1.80	2 (20%)
1	TPO	F	186	1	8,10,11	1.61	1 (12%)	10,14,16	1.89	1 (10%)

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
1	TPO	A	186	1	-	0/9/11/13	-
1	TPO	F	186	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	186	TPO	P-O1P	3.63	1.62	1.50
1	A	186	TPO	P-O1P	3.25	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	186	TPO	P-OG1-CB	-5.38	106.94	123.21
1	A	186	TPO	P-OG1-CB	-4.79	108.73	123.21
1	A	186	TPO	CG2-CB-CA	-2.09	109.05	113.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 20 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
6	SO4	A	404	-	4,4,4	0.27	0	6,6,6	0.09	0
6	SO4	G	304	-	4,4,4	0.27	0	6,6,6	0.19	0
6	SO4	B	304	-	4,4,4	0.28	0	6,6,6	0.25	0
6	SO4	F	405	-	4,4,4	0.31	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	304	SO4	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	319/326 (97%)	0.04	15 (4%) 31 28	25, 59, 112, 130	0
1	F	324/326 (99%)	0.18	21 (6%) 18 14	23, 66, 112, 137	0
2	B	256/266 (96%)	-0.23	5 (1%) 65 63	18, 39, 89, 110	0
2	G	255/266 (95%)	-0.16	9 (3%) 44 38	22, 48, 99, 118	0
3	C	48/48 (100%)	-0.24	0 100 100	23, 42, 61, 83	0
3	H	48/48 (100%)	-0.18	0 100 100	27, 51, 72, 88	0
4	E	38/43 (88%)	-0.05	1 (2%) 56 52	36, 54, 96, 100	0
4	J	38/43 (88%)	0.15	1 (2%) 56 52	58, 75, 108, 114	0
All	All	1326/1366 (97%)	-0.03	52 (3%) 39 35	18, 54, 103, 137	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	30	PHE	6.9
2	G	256	TRP	6.2
1	F	327	MET	6.0
1	A	31	GLY	6.0
1	F	29	THR	5.8
2	G	257	ASN	5.8
1	A	30	PHE	5.7
1	F	31	GLY	5.7
2	G	255	ILE	5.5
1	A	178	LYS	5.4
1	F	331	HIS	5.1
1	F	330	THR	5.1
1	F	22	LEU	4.4
1	A	29	THR	4.4
1	F	27	GLN	4.2
1	A	331	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	28	GLY	4.2
1	F	332	LEU	4.0
2	B	259	ARG	4.0
1	A	330	THR	3.8
1	A	28	GLY	3.6
1	A	181	GLN	3.4
1	A	22	LEU	3.4
2	B	262	GLU	3.4
2	B	256	TRP	3.3
1	F	53	GLU	3.3
2	G	252	LEU	3.2
1	A	25	ILE	3.2
1	F	329	SER	3.2
1	F	55	GLU	3.1
2	G	258	TRP	3.1
1	A	34	PHE	2.9
1	F	326	GLY	2.9
4	J	32	SER	2.8
2	G	253	LYS	2.8
1	F	269	LYS	2.7
4	E	32	SER	2.7
1	A	26	GLY	2.6
2	B	119	PRO	2.6
1	F	93	ASN	2.5
1	F	262	TYR	2.4
1	A	327	MET	2.3
1	A	329	SER	2.3
1	F	25	ILE	2.3
1	A	27	GLN	2.2
1	F	178	LYS	2.2
1	F	26	GLY	2.2
2	G	254	ARG	2.1
2	G	7	ASN	2.1
2	B	7	ASN	2.1
2	G	259	ARG	2.1
1	F	23	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	TPO	A	186	11/12	0.98	0.16	23,36,43,43	0
1	TPO	F	186	11/12	0.98	0.15	29,38,45,52	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	YT3	F	404	1/1	0.65	0.11	138,138,138,138	0
6	SO4	A	404	5/5	0.93	0.24	103,106,107,110	0
6	SO4	F	405	5/5	0.93	0.16	85,90,96,97	0
5	YT3	J	101	1/1	0.94	0.17	105,105,105,105	0
6	SO4	B	304	5/5	0.95	0.11	77,77,78,83	0
5	YT3	G	303	1/1	0.95	0.14	92,92,92,92	0
5	YT3	F	403	1/1	0.96	0.13	106,106,106,106	0
6	SO4	G	304	5/5	0.96	0.18	96,97,99,100	0
5	YT3	E	101	1/1	0.97	0.15	46,46,46,46	0
5	YT3	A	403	1/1	0.98	0.11	76,76,76,76	0
5	YT3	E	102	1/1	0.98	0.11	93,93,93,93	0
5	YT3	G	301	1/1	0.98	0.13	71,71,71,71	0
7	ZN	H	101	1/1	0.98	0.13	46,46,46,46	0
7	ZN	H	102	1/1	0.98	0.09	59,59,59,59	0
5	YT3	F	401	1/1	0.99	0.15	42,42,42,42	0
5	YT3	F	402	1/1	0.99	0.18	59,59,59,59	0
5	YT3	B	302	1/1	0.99	0.15	57,57,57,57	0
5	YT3	B	303	1/1	0.99	0.12	41,41,41,41	0
5	YT3	A	402	1/1	0.99	0.18	87,87,87,87	0
7	ZN	C	102	1/1	0.99	0.11	55,55,55,55	0
5	YT3	G	302	1/1	0.99	0.13	63,63,63,63	0
5	YT3	A	401	1/1	0.99	0.18	65,65,65,65	0
7	ZN	C	101	1/1	1.00	0.12	32,32,32,32	0
5	YT3	B	301	1/1	1.00	0.15	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.