



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SK6  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin, 3',5' cyclic AMP (cAMP), and pyrophosphate  
Authors : Guo, Q.; Shen, Y.; Zhukovskaya, N.L.; Tang, W.J.  
Deposited on : 2004-03-04  
Resolution : 3.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

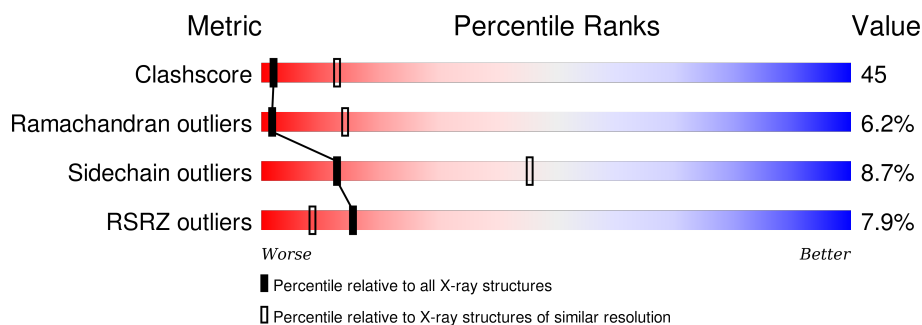
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	510	<div> <div>2%</div> <div>36% 50% 8% 6%</div> </div>
1	B	510	<div> <div>5%</div> <div>23% 52% 12% 11%</div> </div>
1	C	510	<div> <div>4%</div> <div>38% 47% 8% 5%</div> </div>
2	D	148	<div> <div>17%</div> <div>41% 48% 7%</div> </div>
2	E	148	<div> <div>28%</div> <div>45% 41% 11%</div> </div>
2	F	148	<div> <div>17%</div> <div>39% 49% 9%</div> </div>

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
3	CA	D	801	-	-	-	X
3	CA	F	805	-	-	-	X
4	YB	A	907	-	-	-	X
4	YB	B	905	-	-	-	X
4	YB	B	908	-	-	-	X
5	CMP	A	289	X	-	-	-
5	CMP	B	290	X	-	-	-
5	CMP	C	910	X	-	-	-
6	POP	A	893	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15050 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 Calmodulin-sensitive adenylyate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3924	2511	668	742	3			
1	B	454	Total	C	N	O	S	0	0	0
			3706	2370	628	705	3			
1	C	483	Total	C	N	O	S	0	0	0
			3937	2519	670	745	3			

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

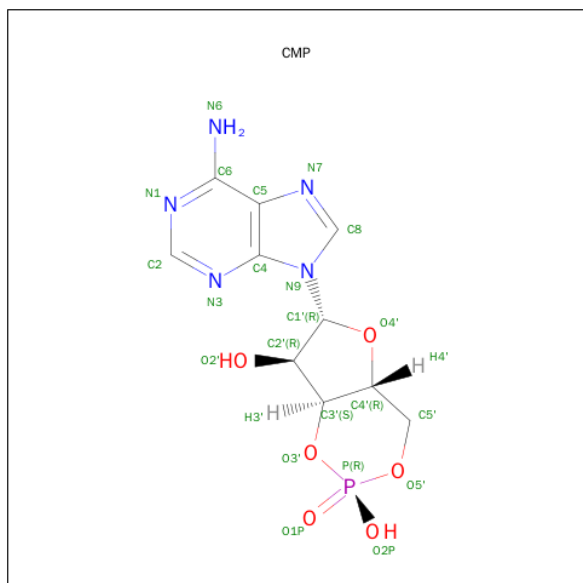
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Yb	0	0
			3	3		

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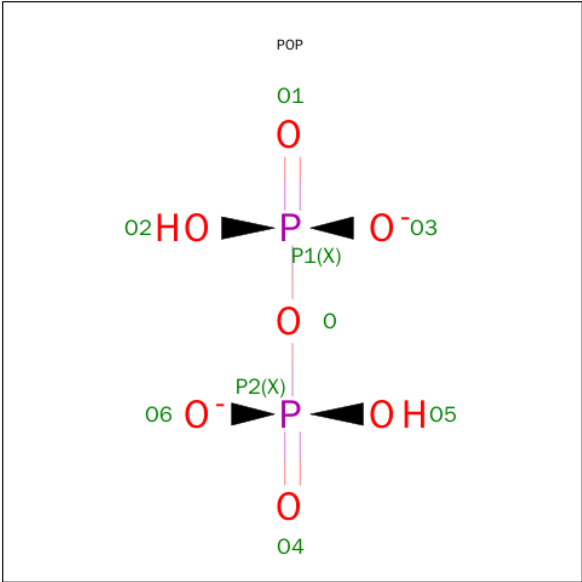
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Yb	0	0
			3	3		
4	C	3	Total	Yb	0	0
			3	3		

- Molecule 5 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula:  $C_{10}H_{12}N_5O_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
5	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
5	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $H_2O_7P_2$ ).

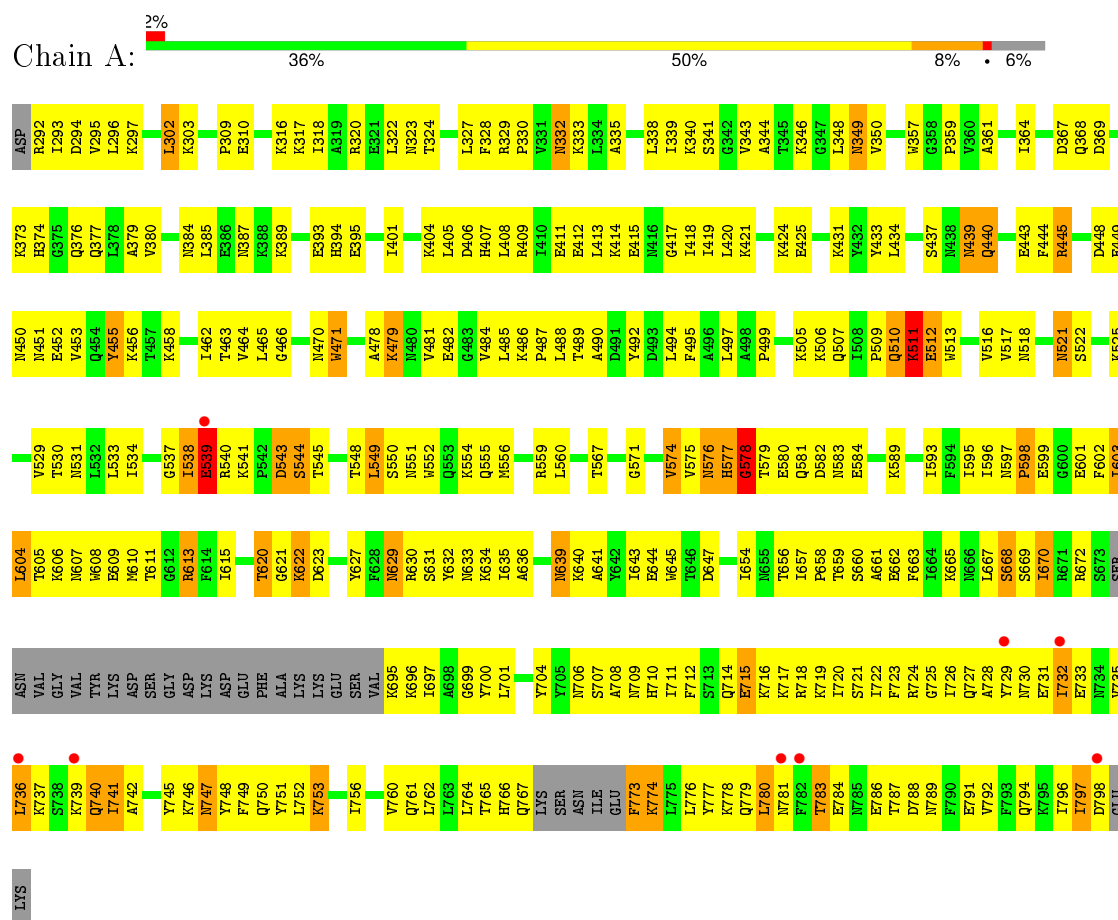


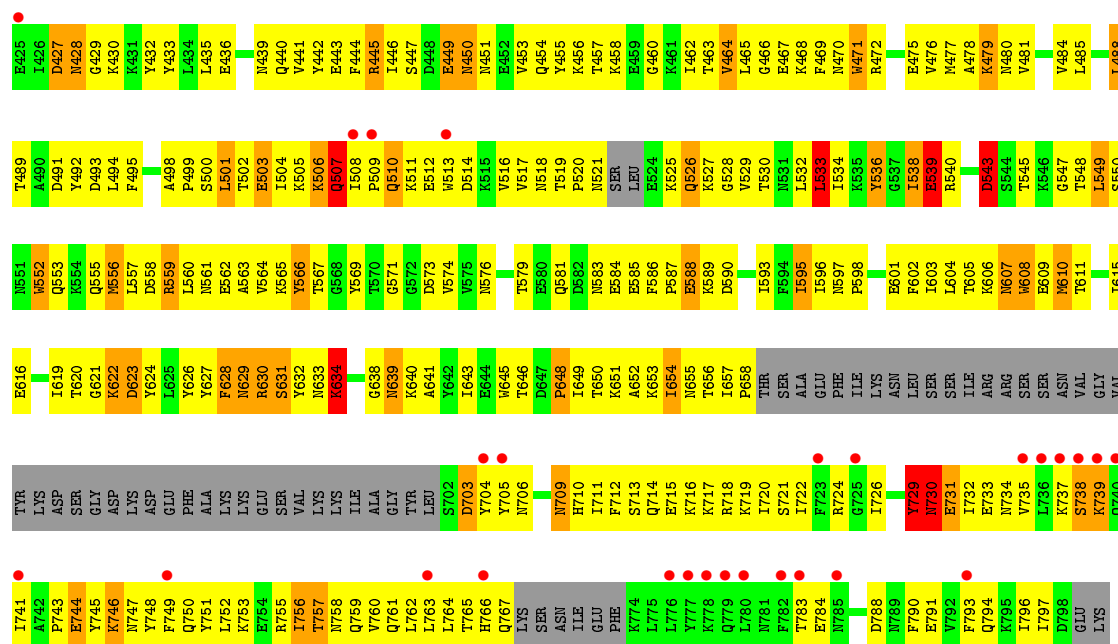
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			9	7	2		
6	B	1	Total	O	P	0	0
			9	7	2		
6	C	1	Total	O	P	0	0
			9	7	2		

### 3 Residue-property plots

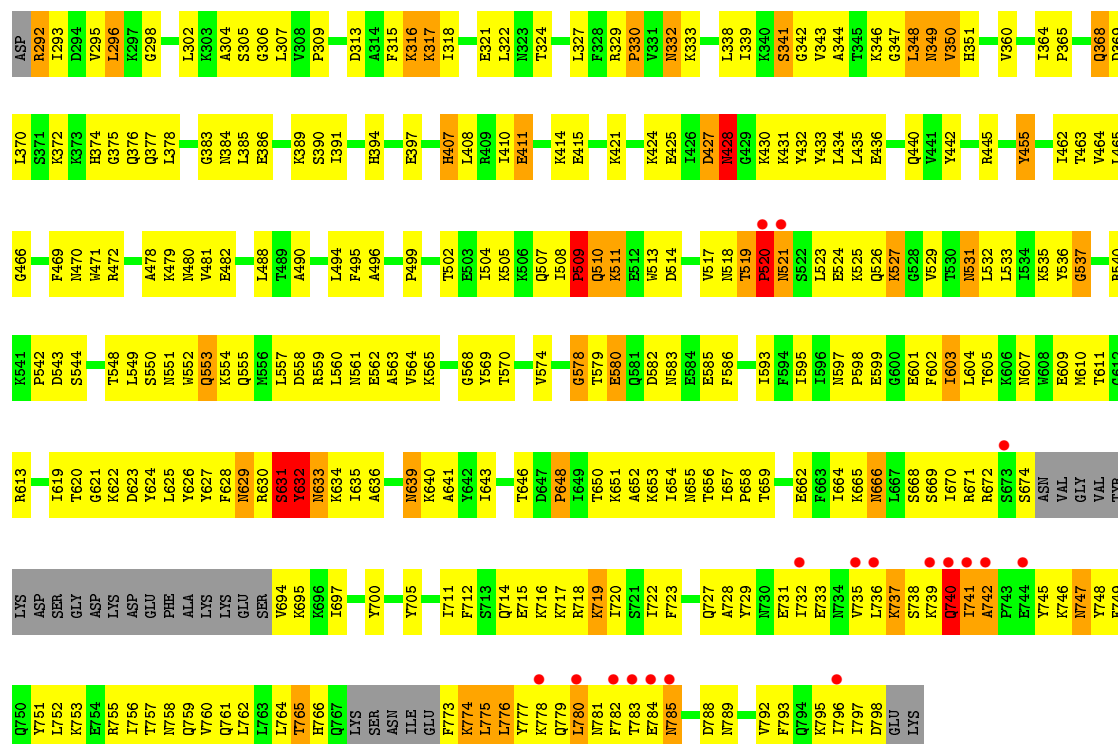
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Calmodulin-sensitive adenylate cyclase

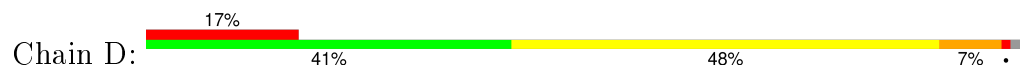




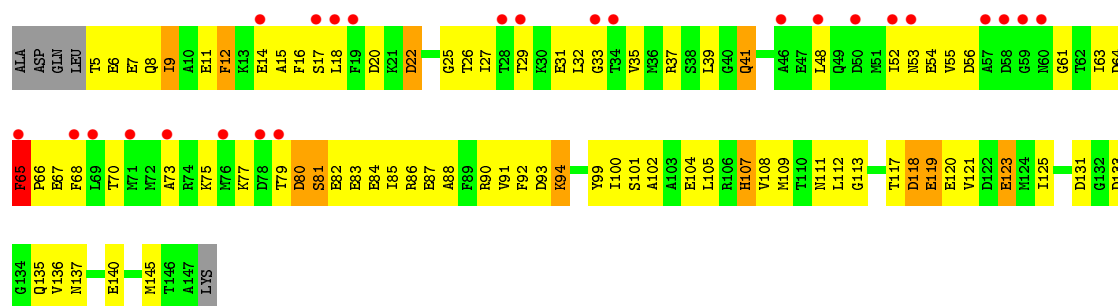
• Molecule 1: Calmodulin-sensitive adenylylate cyclase



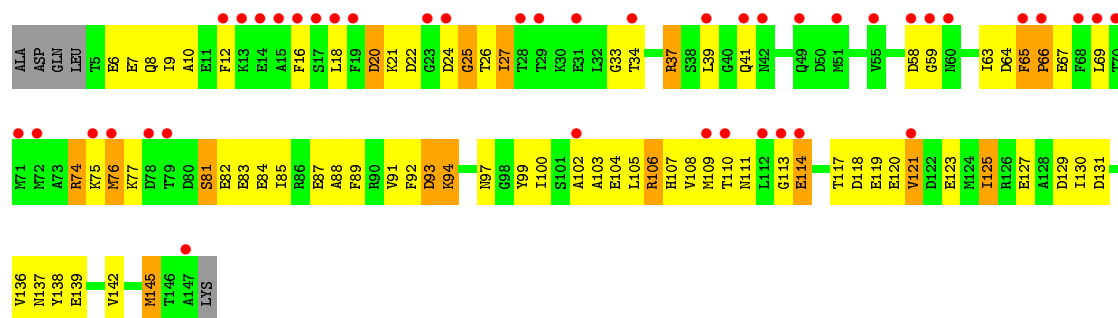
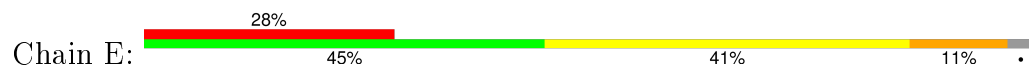
• Molecule 2: Calmodulin



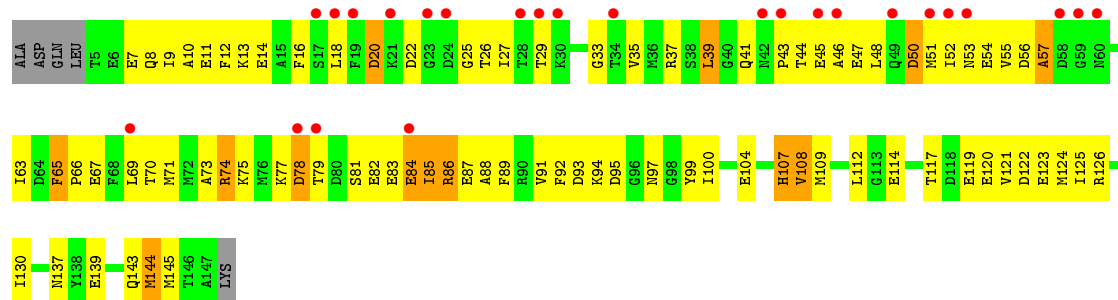
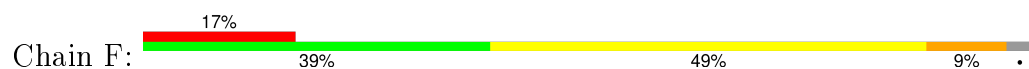




• Molecule 2: Calmodulin



• Molecule 2: Calmodulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.87Å 166.45Å 342.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 43.11 – 3.29	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-3.20) 95.7 (43.11-3.29)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.250 , 0.307 0.268 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50500 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	15050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, YB, POP, CMP

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	0.57	5/3999 (0.1%)	0.91	25/5382 (0.5%)
1	B	0.64	5/3778 (0.1%)	0.97	22/5088 (0.4%)
1	C	0.84	8/4012 (0.2%)	1.30	36/5400 (0.7%)
2	D	0.39	0/1137	0.56	0/1527
2	E	0.36	0/1137	0.54	0/1527
2	F	0.45	1/1137 (0.1%)	0.62	0/1527
All	All	0.64	19/15200 (0.1%)	0.99	83/20451 (0.4%)

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	2
1	B	0	1
1	C	1	5
All	All	1	8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	PRO	N-CD	20.86	1.77	1.47
1	C	773	PHE	C-N	20.19	1.80	1.34
1	C	632	TYR	N-CA	19.71	1.85	1.46
1	C	741	ILE	N-CA	15.98	1.78	1.46
1	C	521	ASN	N-CA	14.19	1.74	1.46
1	B	730	ASN	N-CA	13.64	1.73	1.46
1	A	578	GLY	N-CA	12.15	1.64	1.46
1	A	774	LYS	N-CA	10.20	1.66	1.46
1	C	428	ASN	N-CA	9.03	1.64	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	HIS	N-CA	8.69	1.63	1.46
1	B	622	LYS	N-CA	8.34	1.63	1.46
1	C	511	LYS	N-CA	8.29	1.62	1.46
1	B	471	TRP	N-CA	6.90	1.60	1.46
1	B	738	SER	N-CA	6.41	1.59	1.46
1	A	539	GLU	N-CA	6.16	1.58	1.46
1	C	520	PRO	N-CA	5.98	1.57	1.47
2	F	84	GLU	CB-CG	5.91	1.63	1.52
1	A	543	ASP	C-N	-5.27	1.22	1.34
1	B	797	ILE	N-CA	5.04	1.56	1.46

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	773	PHE	O-C-N	-46.13	48.88	122.70
1	C	773	PHE	CB-CA-C	22.71	155.82	110.40
1	C	773	PHE	N-CA-C	-22.63	49.90	111.00
1	C	520	PRO	CA-N-CD	-18.66	85.37	111.50
1	B	730	ASN	N-CA-CB	-17.00	80.00	110.60
1	C	741	ILE	CB-CA-C	-16.43	78.74	111.60
1	C	511	LYS	N-CA-CB	-15.68	82.38	110.60
1	A	783	THR	CB-CA-C	-15.32	70.23	111.60
1	C	774	LYS	N-CA-CB	-15.27	83.11	110.60
1	A	512	GLU	N-CA-CB	14.57	136.83	110.60
1	B	622	LYS	CB-CA-C	14.47	139.35	110.40
1	C	632	TYR	N-CA-C	-14.43	72.04	111.00
1	C	783	THR	CB-CA-C	-13.66	74.71	111.60
1	B	471	TRP	N-CA-CB	13.62	135.11	110.60
1	C	521	ASN	N-CA-CB	13.57	135.02	110.60
1	C	741	ILE	N-CA-CB	-13.47	79.82	110.80
1	B	423	LYS	N-CA-CB	-12.96	87.27	110.60
1	C	544	SER	N-CA-CB	-12.29	92.06	110.50
1	A	577	HIS	N-CA-CB	-12.16	88.71	110.60
1	A	774	LYS	N-CA-CB	-11.77	89.42	110.60
1	B	622	LYS	N-CA-CB	-11.59	89.75	110.60
1	A	512	GLU	N-CA-C	-11.54	79.84	111.00
1	C	773	PHE	CA-C-N	-11.01	92.98	117.20
1	A	740	GLN	CB-CA-C	-10.34	89.72	110.40
1	C	783	THR	N-CA-C	10.21	138.56	111.00
1	C	631	SER	C-N-CA	-10.05	96.58	121.70
1	B	731	GLU	N-CA-CB	9.81	128.27	110.60
1	C	774	LYS	N-CA-C	9.65	137.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	HIS	C-N-CA	-9.58	102.18	122.30
1	B	623	ASP	N-CA-CB	-9.57	93.38	110.60
1	B	543	ASP	N-CA-CB	-9.25	93.94	110.60
1	A	543	ASP	C-N-CA	-9.15	98.83	121.70
1	B	538	ILE	CB-CA-C	-9.04	93.52	111.60
1	C	428	ASN	N-CA-C	8.83	134.84	111.00
1	A	741	ILE	N-CA-CB	-8.63	90.95	110.80
1	A	784	GLU	N-CA-CB	-8.48	95.34	110.60
1	A	740	GLN	N-CA-C	-8.40	88.31	111.00
1	A	783	THR	N-CA-C	8.29	133.38	111.00
1	C	428	ASN	N-CA-CB	-8.25	95.75	110.60
1	C	519	THR	C-N-CD	-8.21	102.54	120.60
1	C	742	ALA	N-CA-C	8.09	132.83	111.00
1	A	543	ASP	CA-C-N	7.85	134.48	117.20
1	C	509	PRO	CA-N-CD	-7.79	100.60	111.50
1	C	784	GLU	N-CA-CB	-7.77	96.62	110.60
1	C	632	TYR	N-CA-CB	7.75	124.55	110.60
1	B	737	LYS	CB-CA-C	-7.60	95.20	110.40
1	C	784	GLU	N-CA-C	-7.52	90.69	111.00
1	B	797	ILE	N-CA-CB	-7.47	93.61	110.80
1	B	538	ILE	N-CA-C	7.42	131.02	111.00
1	C	741	ILE	N-CA-C	-7.32	91.23	111.00
1	B	703	ASP	N-CA-CB	-7.21	97.62	110.60
1	C	520	PRO	C-N-CA	-7.05	104.07	121.70
1	A	539	GLU	CA-C-N	-7.04	101.71	117.20
1	B	507	GLN	N-CA-CB	-7.03	97.95	110.60
1	C	740	GLN	C-N-CA	-6.97	104.26	121.70
1	C	773	PHE	C-N-CA	-6.97	104.28	121.70
1	A	511	LYS	C-N-CA	6.88	138.90	121.70
1	C	785	ASN	N-CA-CB	-6.80	98.36	110.60
1	B	729	TYR	C-N-CA	-6.78	104.75	121.70
1	C	520	PRO	CA-C-N	-6.64	102.59	117.20
1	B	738	SER	N-CA-C	-6.62	93.13	111.00
1	A	544	SER	CA-C-N	-6.38	103.17	117.20
1	C	624	TYR	N-CA-CB	6.36	122.05	110.60
1	A	576	ASN	C-N-CA	-6.16	106.29	121.70
1	A	784	GLU	N-CA-C	-6.09	94.55	111.00
1	A	543	ASP	O-C-N	-6.08	112.97	122.70
1	A	543	ASP	N-CA-C	-5.89	95.09	111.00
1	B	737	LYS	C-N-CA	-5.77	107.28	121.70
1	A	786	GLU	N-CA-CB	-5.70	100.34	110.60
1	B	323	ASN	N-CA-CB	-5.64	100.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	786	GLU	N-CA-C	5.63	126.20	111.00
1	B	730	ASN	N-CA-C	5.54	125.97	111.00
1	B	471	TRP	N-CA-C	-5.48	96.19	111.00
1	A	538	ILE	N-CA-CB	-5.45	98.26	110.80
1	C	520	PRO	N-CA-C	-5.38	98.11	112.10
1	B	539	GLU	N-CA-C	-5.31	96.66	111.00
1	C	634	LYS	N-CA-C	-5.17	97.05	111.00
1	C	624	TYR	N-CA-C	-5.15	97.09	111.00
1	C	775	LEU	N-CA-CB	-5.12	100.17	110.40
1	C	543	ASP	N-CA-CB	5.10	119.78	110.60
1	A	539	GLU	C-N-CA	5.07	134.38	121.70
1	B	533	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	539	GLU	O-C-N	5.00	130.70	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	773	PHE	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	LYS	Peptide
1	A	773	PHE	Peptide
1	B	729	TYR	Peptide
1	C	427	ASP	Peptide
1	C	510	GLN	Peptide
1	C	520	PRO	Peptide
1	C	631	SER	Peptide
1	C	740	GLN	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	3924	0	3967	345	0
1	B	3706	0	3728	472	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3937	0	3980	329	0
2	D	1125	0	1049	82	0
2	E	1125	0	1049	92	0
2	F	1125	0	1048	102	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
5	A	22	0	10	6	0
5	B	22	0	10	5	0
5	C	22	0	10	3	0
6	A	9	0	0	3	0
6	B	9	0	0	1	0
6	C	9	0	0	1	0
All	All	15050	0	14851	1356	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1356) 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)
5:B:290:CMP:C2	5:B:290:CMP:H2	0.97	1.49
5:A:289:CMP:H2	5:A:289:CMP:C2	0.97	1.48
5:C:910:CMP:C2	5:C:910:CMP:H2	0.97	1.47
1:B:730:ASN:CA	1:B:730:ASN:N	1.73	1.46
1:C:741:ILE:CA	1:C:741:ILE:N	1.78	1.46
1:C:521:ASN:CA	1:C:521:ASN:N	1.74	1.45
1:C:520:PRO:CD	1:C:520:PRO:N	1.77	1.38
1:C:632:TYR:N	1:C:632:TYR:CA	1.85	1.36
1:C:632:TYR:N	1:C:632:TYR:C	2.00	1.14
1:B:730:ASN:N	1:B:730:ASN:CB	2.11	1.13
1:B:322:LEU:O	1:B:324:THR:HG22	1.49	1.13
1:B:657:ILE:HG13	1:B:658:PRO:HD2	1.23	1.12
1:B:538:ILE:HG22	1:B:538:ILE:O	1.47	1.12
1:C:632:TYR:N	1:C:632:TYR:O	1.83	1.11
1:C:741:ILE:CB	1:C:741:ILE:N	2.14	1.10
1:B:326:ILE:HB	1:B:596:ILE:HB	1.32	1.09
1:B:654:ILE:HA	1:B:755:ARG:HG2	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:GLU:HG2	1:B:734:ASN:H	1.24	1.00
1:A:697:ILE:HD13	1:A:732:ILE:HG12	1.46	0.97
1:A:295:VAL:HG21	1:A:603:ILE:HG22	1.44	0.97
1:B:320:ARG:HG2	1:B:598:PRO:O	1.62	0.96
1:C:671:ARG:HD2	1:C:745:TYR:OH	1.64	0.96
1:B:761:GLN:HA	1:B:764:LEU:HB2	1.44	0.96
1:A:338:LEU:HG	1:A:343:VAL:HG21	1.49	0.94
1:B:548:THR:H	5:B:290:CMP:HN62	0.97	0.94
1:B:439:ASN:ND2	1:B:442:TYR:H	1.66	0.94
1:A:773:PHE:HA	1:A:776:LEU:HD13	1.50	0.93
1:B:456:LYS:HB3	1:B:471:TRP:H	1.32	0.92
1:B:717:LYS:HA	1:B:720:ILE:HG12	1.51	0.92
1:B:548:THR:N	5:B:290:CMP:HN62	1.68	0.92
1:C:633:ASN:N	1:C:633:ASN:HD22	1.64	0.92
1:C:509:PRO:O	1:C:511:LYS:N	2.04	0.90
2:F:85:ILE:HG22	2:F:86:ARG:N	1.87	0.89
1:B:706:ASN:HB3	1:B:709:ASN:HB2	1.53	0.89
1:C:631:SER:C	1:C:632:TYR:CA	2.40	0.88
1:B:456:LYS:HB3	1:B:471:TRP:N	1.88	0.88
1:B:747:ASN:HA	1:B:750:GLN:HB2	1.55	0.88
1:A:349:ASN:H	1:A:349:ASN:HD22	1.19	0.88
1:A:376:GLN:O	1:A:380:VAL:HG23	1.74	0.87
1:B:294:ASP:HB3	1:B:606:LYS:NZ	1.90	0.87
1:B:710:HIS:HB2	2:E:127:GLU:HA	1.57	0.86
1:B:406:ASP:OD2	1:B:408:LEU:HB3	1.74	0.86
1:C:520:PRO:C	1:C:521:ASN:CA	2.43	0.86
1:B:324:THR:HB	1:B:499:PRO:HA	1.55	0.86
1:C:537:GLY:O	1:C:625:LEU:HD21	1.76	0.86
1:C:519:THR:C	1:C:520:PRO:CD	2.44	0.85
1:B:741:ILE:HG21	1:B:745:TYR:HB2	1.56	0.85
1:A:607:ASN:ND2	1:A:609:GLU:HB2	1.91	0.85
1:B:729:TYR:C	1:B:730:ASN:CA	2.44	0.85
1:C:739:LYS:O	1:C:741:ILE:N	2.10	0.85
1:B:632:TYR:O	1:B:634:LYS:HD2	1.77	0.84
1:A:697:ILE:HG12	1:A:731:GLU:HB3	1.59	0.84
1:A:629:ASN:HD22	1:A:631:SER:H	1.26	0.84
1:B:657:ILE:CG1	1:B:658:PRO:HD2	2.05	0.84
1:B:616:GLU:HA	1:B:620:THR:HG22	1.60	0.83
1:C:740:GLN:C	1:C:741:ILE:CA	2.47	0.83
1:B:733:GLU:CG	1:B:734:ASN:H	1.91	0.83
1:B:327:LEU:HD11	1:B:595:ILE:HG23	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:HH21	1:B:588:GLU:HB3	1.44	0.82
1:C:605:THR:HG21	1:C:611:THR:HA	1.60	0.82
1:B:730:ASN:N	1:B:730:ASN:HB2	1.94	0.82
2:F:92:PHE:HA	2:F:108:VAL:HG21	1.59	0.82
1:B:450:ASN:HD22	1:B:450:ASN:H	1.28	0.82
2:E:88:ALA:HA	2:E:91:VAL:HG23	1.62	0.81
1:A:548:THR:H	5:A:289:CMP:HN62	1.26	0.81
1:B:327:LEU:CD1	1:B:595:ILE:HG23	2.10	0.81
1:C:740:GLN:O	1:C:741:ILE:C	2.19	0.81
1:C:716:LYS:O	1:C:720:ILE:HG12	1.79	0.81
1:A:401:ILE:HD11	1:A:487:PRO:HB3	1.61	0.80
1:B:316:LYS:HD2	1:B:317:LYS:N	1.96	0.80
1:A:607:ASN:HD21	1:A:609:GLU:HB2	1.46	0.80
1:B:430:LYS:HD2	1:B:449:GLU:OE2	1.82	0.80
1:C:372:LYS:HE3	6:C:895:POP:O3	1.82	0.80
1:A:349:ASN:ND2	1:A:349:ASN:H	1.79	0.80
1:C:304:ALA:HB3	1:C:604:LEU:HD13	1.65	0.79
2:D:65:PHE:HB2	2:D:66:PRO:HD3	1.64	0.79
1:C:621:GLY:HA2	2:F:94:LYS:HB2	1.62	0.79
2:D:41:GLN:NE2	2:D:75:LYS:HD2	1.97	0.79
1:C:514:ASP:HA	1:C:517:VAL:HG12	1.65	0.79
1:C:540:ARG:HD2	1:C:582:ASP:OD1	1.83	0.79
1:B:605:THR:HG21	1:B:611:THR:HA	1.63	0.78
1:A:797:ILE:HG13	1:A:798:ASP:H	1.49	0.78
1:B:657:ILE:HG13	1:B:658:PRO:CD	2.10	0.78
1:B:631:SER:O	1:B:634:LYS:HG2	1.84	0.78
1:C:550:SER:OG	1:C:553:GLN:HB2	1.84	0.78
1:A:327:LEU:HG	1:A:595:ILE:HG23	1.64	0.78
1:B:294:ASP:O	1:B:606:LYS:HD3	1.84	0.78
1:A:539:GLU:HB2	2:D:84:GLU:HG2	1.65	0.78
2:E:26:THR:HA	2:E:63:ILE:O	1.83	0.78
1:C:427:ASP:O	1:C:428:ASN:HB2	1.83	0.77
1:C:741:ILE:C	1:C:741:ILE:N	2.37	0.77
1:B:443:GLU:HG3	1:B:458:LYS:HD3	1.64	0.77
1:B:605:THR:CG2	1:B:611:THR:HA	2.15	0.77
1:B:366:PHE:HD1	1:B:477:MET:HE1	1.50	0.77
2:D:63:ILE:HA	2:D:67:GLU:OE2	1.84	0.77
1:A:521:ASN:ND2	1:A:522:SER:H	1.83	0.76
1:B:329:ARG:HG3	1:B:330:PRO:HD2	1.68	0.76
1:A:603:ILE:HD12	1:A:603:ILE:N	1.99	0.76
1:B:593:ILE:HG13	1:B:611:THR:HG21	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:THR:HG21	1:B:611:THR:HG23	1.68	0.76
1:C:739:LYS:C	1:C:741:ILE:N	2.39	0.76
1:C:636:ALA:O	1:C:640:LYS:HA	1.86	0.76
1:C:629:ASN:HD22	1:C:631:SER:H	1.34	0.76
1:B:463:THR:HG22	1:B:465:LEU:H	1.51	0.75
1:B:733:GLU:HG2	1:B:734:ASN:N	1.97	0.75
1:A:329:ARG:HD2	1:A:580:GLU:HG3	1.67	0.75
1:C:736:LEU:HD12	1:C:746:LYS:HE2	1.68	0.75
1:B:348:LEU:O	1:B:348:LEU:HD23	1.86	0.75
1:B:500:SER:HA	1:B:624:TYR:CD1	2.22	0.74
1:A:540:ARG:HD2	1:A:582:ASP:OD1	1.86	0.74
1:B:318:ILE:O	1:B:322:LEU:HD23	1.86	0.74
2:F:27:ILE:HG13	2:F:63:ILE:HD12	1.70	0.74
1:A:551:ASN:O	1:A:555:GLN:HG3	1.87	0.74
1:B:445:ARG:HG2	1:B:471:TRP:CH2	2.22	0.74
1:B:720:ILE:HD12	1:B:724:ARG:NH2	2.02	0.74
1:B:649:ILE:HD11	2:E:89:PHE:HD2	1.53	0.74
1:A:462:ILE:HD11	1:A:466:GLY:HA2	1.70	0.74
1:B:345:THR:HG23	1:B:491:ASP:HB3	1.68	0.74
1:A:603:ILE:HD12	1:A:603:ILE:H	1.53	0.73
1:B:326:ILE:HG21	1:B:596:ILE:HD12	1.71	0.73
1:B:329:ARG:HH21	1:B:588:GLU:CB	2.01	0.73
1:A:548:THR:N	5:A:289:CMP:N6	2.36	0.73
2:F:93:ASP:HA	2:F:104:GLU:OE2	1.89	0.73
1:B:648:PRO:O	1:B:651:LYS:HB3	1.89	0.73
2:E:105:LEU:HD23	2:E:105:LEU:O	1.88	0.73
2:D:15:ALA:O	2:D:18:LEU:HG	1.89	0.72
1:A:621:GLY:O	1:A:622:LYS:HE2	1.88	0.72
1:C:741:ILE:HB	1:C:741:ILE:N	2.01	0.72
1:B:335:ALA:O	1:B:339:ILE:HG13	1.88	0.72
1:A:344:ALA:O	1:A:489:THR:HG22	1.89	0.72
1:B:445:ARG:HG2	1:B:471:TRP:CZ3	2.24	0.72
1:A:747:ASN:OD1	1:B:397:GLU:HG3	1.87	0.72
1:B:294:ASP:OD1	1:B:606:LYS:HD2	1.90	0.72
1:A:445:ARG:HD2	1:A:471:TRP:CZ2	2.23	0.72
1:B:716:LYS:O	1:B:720:ILE:HG23	1.89	0.72
2:E:119:GLU:O	2:E:123:GLU:HB2	1.90	0.72
1:C:424:LYS:CD	1:C:431:LYS:HE3	2.19	0.72
1:B:726:ILE:HA	1:B:729:TYR:HE2	1.54	0.72
1:A:295:VAL:CG2	1:A:603:ILE:HG22	2.18	0.72
1:B:712:PHE:HD2	1:B:716:LYS:HG2	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:ILE:HD12	1:B:724:ARG:HH21	1.55	0.72
1:B:539:GLU:HG2	2:E:84:GLU:HG2	1.71	0.71
1:B:602:PHE:O	1:B:603:ILE:HD13	1.89	0.71
1:B:506:LYS:HG2	1:B:506:LYS:O	1.89	0.71
1:A:715:GLU:O	1:A:719:LYS:HG2	1.89	0.71
2:F:51:MET:O	2:F:54:GLU:HB3	1.90	0.71
1:C:697:ILE:HG13	1:C:731:GLU:OE1	1.90	0.71
1:A:525:LYS:O	1:A:529:VAL:HG23	1.91	0.71
1:B:548:THR:N	5:B:290:CMP:N6	2.33	0.71
1:C:629:ASN:ND2	1:C:631:SER:H	1.89	0.71
1:C:739:LYS:C	1:C:741:ILE:H	1.95	0.71
1:A:654:ILE:O	1:A:654:ILE:HG12	1.90	0.71
2:E:88:ALA:HA	2:E:91:VAL:CG2	2.21	0.70
1:C:313:ASP:O	1:C:316:LYS:HB2	1.92	0.70
1:B:714:GLN:CD	1:B:714:GLN:H	1.94	0.70
1:B:539:GLU:CD	2:E:84:GLU:CD	2.50	0.70
1:B:338:LEU:HB3	1:B:343:VAL:HG21	1.73	0.70
1:B:450:ASN:ND2	1:B:450:ASN:H	1.90	0.70
1:B:649:ILE:HD11	2:E:89:PHE:CD2	2.27	0.70
2:E:65:PHE:HB2	2:E:66:PRO:HD3	1.74	0.70
1:A:349:ASN:N	1:A:349:ASN:HD22	1.79	0.70
1:B:463:THR:HG22	1:B:465:LEU:N	2.07	0.69
1:C:505:LYS:HD3	2:F:112:LEU:O	1.92	0.69
1:A:346:LYS:HD3	6:A:893:POP:O2	1.92	0.69
1:A:541:LYS:HB2	1:A:541:LYS:NZ	2.07	0.69
1:B:512:GLU:O	1:B:516:VAL:HG22	1.92	0.69
1:B:509:PRO:HB2	1:B:511:LYS:HD3	1.75	0.69
1:A:318:ILE:N	1:A:318:ILE:HD12	2.07	0.69
1:B:538:ILE:CG2	1:B:538:ILE:O	2.14	0.69
1:A:629:ASN:ND2	1:A:631:SER:H	1.88	0.69
1:A:577:HIS:CG	1:A:577:HIS:O	2.45	0.69
1:C:540:ARG:HD3	1:C:627:TYR:OH	1.92	0.69
1:A:667:LEU:HB3	2:D:14:GLU:OE2	1.93	0.69
1:B:390:SER:HB3	1:B:398:ILE:HG21	1.73	0.69
1:B:439:ASN:HD21	1:B:442:TYR:H	1.37	0.68
1:A:540:ARG:NH2	1:A:630:ARG:NH2	2.41	0.68
1:B:427:ASP:C	1:B:429:GLY:H	1.96	0.68
1:B:550:SER:OG	1:B:553:GLN:HG3	1.93	0.68
1:A:540:ARG:NH1	1:A:627:TYR:CE1	2.61	0.68
1:B:326:ILE:C	1:B:327:LEU:HD22	2.13	0.68
1:C:521:ASN:N	1:C:521:ASN:C	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:THR:HG21	1:A:611:THR:HA	1.76	0.68
1:A:322:LEU:O	1:A:324:THR:HG23	1.93	0.68
1:B:332:ASN:HD22	1:B:333:LYS:N	1.92	0.68
1:B:757:THR:O	1:B:760:VAL:HG22	1.94	0.68
1:B:744:GLU:HG2	1:C:397:GLU:OE1	1.93	0.68
1:C:715:GLU:O	1:C:719:LYS:HG2	1.93	0.68
2:E:102:ALA:HB1	2:E:121:VAL:HG12	1.75	0.68
1:B:519:THR:N	1:B:520:PRO:HD3	2.08	0.68
1:B:372:LYS:HE3	6:B:894:POP:O6	1.94	0.68
1:B:561:ASN:O	1:B:564:VAL:HG22	1.94	0.67
1:C:748:TYR:O	1:C:751:TYR:HB3	1.94	0.67
1:B:469:PHE:HB2	1:B:472:ARG:HD2	1.76	0.67
1:B:414:LYS:HB3	1:B:414:LYS:HZ2	1.59	0.67
1:A:296:LEU:HD12	1:A:604:LEU:HD22	1.76	0.67
1:A:657:ILE:HD11	1:A:704:TYR:CD1	2.30	0.67
1:A:629:ASN:HD22	1:A:631:SER:N	1.93	0.67
1:A:490:ALA:HA	6:A:893:POP:O2	1.95	0.67
1:C:462:ILE:HD11	1:C:466:GLY:HA2	1.77	0.67
1:B:419:ILE:HD12	1:B:435:LEU:HG	1.75	0.67
1:B:312:ALA:O	1:B:315:PHE:HB2	1.93	0.67
1:C:327:LEU:HD23	1:C:595:ILE:HG12	1.77	0.67
1:B:505:LYS:O	1:B:507:GLN:N	2.25	0.67
1:C:785:ASN:HA	1:C:789:ASN:OD1	1.95	0.67
2:E:7:GLU:C	2:E:9:ILE:H	1.98	0.67
1:A:373:LYS:HD2	1:A:379:ALA:HB1	1.77	0.67
1:C:781:ASN:ND2	1:C:789:ASN:HA	2.10	0.66
1:C:597:ASN:HB2	1:C:598:PRO:HD2	1.76	0.66
1:A:463:THR:HG22	1:A:465:LEU:H	1.60	0.66
1:A:722:ILE:HD13	1:A:764:LEU:HG	1.75	0.66
1:A:497:LEU:HD13	1:A:556:MET:HG2	1.77	0.66
1:B:294:ASP:HB3	1:B:606:LYS:HZ3	1.59	0.66
1:B:761:GLN:O	1:B:765:THR:HG23	1.96	0.66
1:A:481:VAL:HG23	1:A:481:VAL:O	1.94	0.66
1:B:539:GLU:OE2	2:E:84:GLU:CD	2.34	0.66
1:B:517:VAL:HG22	2:E:114:GLU:OE2	1.96	0.66
1:C:508:ILE:HG12	1:C:536:TYR:HD2	1.61	0.66
1:B:706:ASN:HB3	1:B:709:ASN:CB	2.24	0.66
1:B:562:GLU:HA	1:B:565:LYS:HD3	1.77	0.66
1:A:593:ILE:HG13	1:A:611:THR:HG21	1.76	0.66
1:A:404:LYS:HE2	1:A:452:GLU:HG2	1.78	0.66
1:A:736:LEU:HD21	1:A:749:PHE:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:LYS:HB2	2:F:18:LEU:HB3	1.78	0.66
1:B:561:ASN:O	1:B:565:LYS:HG3	1.96	0.65
1:B:717:LYS:HA	1:B:720:ILE:CG1	2.26	0.65
1:A:739:LYS:HE3	1:A:740:GLN:O	1.94	0.65
1:B:327:LEU:N	1:B:327:LEU:HD22	2.12	0.65
1:B:649:ILE:HD12	1:B:649:ILE:N	2.11	0.65
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.79	0.65
1:C:718:ARG:O	1:C:722:ILE:HG13	1.97	0.65
1:B:711:ILE:HG13	1:B:712:PHE:HD1	1.60	0.65
2:F:83:GLU:C	2:F:85:ILE:N	2.49	0.65
1:B:730:ASN:O	1:B:733:GLU:HB3	1.96	0.65
1:B:414:LYS:HB3	1:B:414:LYS:NZ	2.11	0.65
1:A:697:ILE:HD13	1:A:732:ILE:CG1	2.25	0.65
1:B:386:GLU:HA	1:B:389:LYS:HE2	1.78	0.65
1:C:639:ASN:ND2	1:C:641:ALA:H	1.95	0.65
1:A:479:LYS:HB2	1:A:488:LEU:HD21	1.79	0.65
1:C:776:LEU:HD23	1:C:779:GLN:NE2	2.12	0.65
2:F:95:ASP:OD1	2:F:104:GLU:OE2	2.14	0.65
2:E:138:TYR:O	2:E:142:VAL:HG23	1.95	0.65
1:B:471:TRP:HA	1:B:471:TRP:CE3	2.33	0.65
1:B:706:ASN:CB	1:B:709:ASN:HB2	2.27	0.65
1:B:608:TRP:CZ2	1:B:643:ILE:HG21	2.31	0.65
1:C:607:ASN:OD1	1:C:610:MET:HB3	1.97	0.65
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.79	0.65
2:E:41:GLN:HE22	2:E:75:LYS:HD2	1.61	0.65
2:F:83:GLU:OE1	2:F:83:GLU:HA	1.98	0.64
2:F:95:ASP:OD1	2:F:97:ASN:OD1	2.14	0.64
1:B:427:ASP:O	1:B:429:GLY:N	2.30	0.64
1:A:521:ASN:CG	1:A:522:SER:H	2.01	0.64
1:B:616:GLU:HA	1:B:620:THR:CG2	2.26	0.64
1:C:424:LYS:HD2	1:C:431:LYS:HE3	1.79	0.64
1:B:462:ILE:HD12	1:B:466:GLY:HA2	1.78	0.64
1:B:391:ILE:CD1	1:B:399:GLY:HA2	2.27	0.64
1:C:764:LEU:O	1:C:766:HIS:N	2.28	0.64
1:A:348:LEU:HD12	1:A:545:THR:O	1.98	0.64
1:C:529:VAL:HG11	2:F:109:MET:SD	2.36	0.64
1:B:508:ILE:HG21	1:B:532:LEU:HD21	1.80	0.64
1:C:607:ASN:O	1:C:610:MET:N	2.29	0.64
1:C:653:LYS:O	1:C:755:ARG:HD3	1.97	0.64
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.80	0.64
1:C:526:GLN:HB3	2:F:124:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:THR:HB	1:B:467:GLU:H	1.63	0.64
2:E:92:PHE:CE2	2:E:108:VAL:HG11	2.34	0.63
1:C:603:ILE:HD12	1:C:603:ILE:N	2.13	0.63
2:E:75:LYS:C	2:E:77:LYS:H	2.01	0.63
1:A:622:LYS:O	1:A:623:ASP:HB2	1.99	0.63
1:C:463:THR:HG22	1:C:465:LEU:H	1.63	0.63
1:B:400:LYS:HD2	1:B:475:GLU:OE1	1.99	0.63
1:C:351:HIS:HB2	1:C:386:GLU:OE1	1.99	0.63
1:B:470:ASN:ND2	1:B:470:ASN:O	2.31	0.63
2:D:93:ASP:HA	2:D:104:GLU:OE2	1.99	0.63
1:A:719:LYS:HE2	1:A:767:GLN:HE21	1.64	0.63
1:C:295:VAL:HG23	1:C:605:THR:HA	1.81	0.63
1:B:332:ASN:C	1:B:332:ASN:HD22	2.02	0.63
1:B:565:LYS:C	1:B:567:THR:H	2.02	0.63
1:A:750:GLN:HG3	1:A:751:TYR:N	2.13	0.63
1:A:539:GLU:HG2	2:D:84:GLU:OE1	1.99	0.63
1:C:741:ILE:H	1:C:741:ILE:HG12	1.64	0.62
1:A:317:LYS:HB3	1:A:318:ILE:HD12	1.80	0.62
1:B:480:ASN:HA	1:B:485:LEU:HD12	1.81	0.62
1:C:697:ILE:HG12	1:C:731:GLU:HB3	1.81	0.62
1:A:510:GLN:O	1:A:510:GLN:HG3	1.99	0.62
1:A:302:LEU:HD11	1:A:309:PRO:HA	1.80	0.62
1:C:732:ILE:O	1:C:736:LEU:HD23	1.99	0.62
2:D:92:PHE:HA	2:D:108:VAL:HG21	1.82	0.62
1:A:513:TRP:O	1:A:517:VAL:HG23	1.99	0.62
1:C:671:ARG:HG3	1:C:674:SER:HB2	1.81	0.62
1:B:713:SER:O	1:B:716:LYS:HB3	2.00	0.62
1:C:728:ALA:O	1:C:732:ILE:HG13	2.00	0.62
1:C:633:ASN:N	1:C:633:ASN:ND2	2.38	0.62
1:C:295:VAL:HB	1:C:610:MET:HE1	1.81	0.62
1:A:779:GLN:HG3	1:A:780:LEU:N	2.15	0.62
1:B:308:VAL:O	1:B:311:HIS:HB2	2.00	0.62
1:C:631:SER:O	1:C:632:TYR:CA	2.47	0.62
1:B:322:LEU:HB2	1:B:503:GLU:OE1	2.00	0.62
1:B:615:ILE:HD12	1:B:645:TRP:HH2	1.65	0.62
1:C:797:ILE:HG13	1:C:798:ASP:H	1.63	0.62
1:C:368:GLN:HG3	1:C:383:GLY:C	2.19	0.62
1:A:424:LYS:HG3	1:A:431:LYS:HD2	1.82	0.62
1:A:548:THR:N	5:A:289:CMP:HN62	1.96	0.62
1:B:322:LEU:HG	1:B:322:LEU:O	2.00	0.62
1:A:647:ASP:OD2	2:D:90:ARG:NE	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:LYS:HD3	1:C:527:LYS:C	2.20	0.62
2:E:94:LYS:NZ	2:E:94:LYS:HB2	2.15	0.62
1:A:583:ASN:ND2	5:A:289:CMP:O4'	2.32	0.61
1:B:649:ILE:C	1:B:651:LYS:H	2.01	0.61
1:A:777:TYR:CD1	1:A:780:LEU:HD11	2.35	0.61
2:D:41:GLN:CD	2:D:75:LYS:HD2	2.21	0.61
1:B:479:LYS:HG3	1:B:480:ASN:N	2.14	0.61
1:A:718:ARG:O	1:A:722:ILE:HG13	2.00	0.61
2:D:22:ASP:OD2	2:D:26:THR:N	2.33	0.61
1:A:450:ASN:O	1:A:451:ASN:HB2	2.00	0.61
2:F:117:THR:OG1	2:F:120:GLU:HG3	2.00	0.61
1:A:661:ALA:HB1	1:A:665:LYS:NZ	2.16	0.61
1:C:740:GLN:C	1:C:741:ILE:C	2.58	0.61
1:B:655:ASN:HA	1:B:759:GLN:NE2	2.15	0.61
1:A:732:ILE:HG22	1:A:732:ILE:O	2.01	0.61
1:B:721:SER:HA	1:B:724:ARG:HG2	1.81	0.61
1:C:430:LYS:HA	1:C:430:LYS:HE2	1.82	0.61
1:A:766:HIS:HB2	1:A:767:GLN:OE1	2.01	0.61
1:C:295:VAL:O	1:C:295:VAL:HG13	2.00	0.61
1:A:505:LYS:HD3	2:D:112:LEU:O	2.00	0.61
1:C:741:ILE:CG1	1:C:741:ILE:N	2.63	0.61
1:C:427:ASP:O	1:C:428:ASN:CB	2.49	0.61
1:C:778:LYS:HB3	1:C:778:LYS:NZ	2.16	0.61
2:E:81:SER:O	2:E:83:GLU:N	2.34	0.60
1:C:789:ASN:HD22	1:C:789:ASN:N	1.99	0.60
2:D:22:ASP:CG	2:D:26:THR:N	2.54	0.60
1:B:560:LEU:O	1:B:563:ALA:HB3	2.00	0.60
1:A:394:HIS:O	1:A:395:GLU:C	2.38	0.60
1:B:565:LYS:O	1:B:567:THR:N	2.34	0.60
1:A:296:LEU:HD12	1:A:604:LEU:CD2	2.31	0.60
1:B:338:LEU:HD21	1:B:363:TYR:CE1	2.37	0.60
1:A:779:GLN:HG3	1:A:780:LEU:H	1.67	0.60
1:A:310:GLU:HG3	1:A:340:LYS:NZ	2.17	0.60
1:C:329:ARG:HD2	1:C:580:GLU:HG3	1.83	0.60
1:A:773:PHE:HD1	1:A:776:LEU:HB2	1.66	0.60
1:B:510:GLN:C	1:B:511:LYS:HD2	2.21	0.60
2:D:20:ASP:OD2	2:D:22:ASP:HB3	2.01	0.60
1:A:443:GLU:HG3	1:A:458:LYS:HG2	1.82	0.60
1:A:756:ILE:O	1:A:760:VAL:HG23	2.02	0.60
1:C:723:PHE:HB2	1:C:793:PHE:CE2	2.37	0.60
1:C:568:GLY:O	1:C:570:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:VAL:C	2:F:123:GLU:H	2.04	0.60
1:A:764:LEU:HD13	1:A:773:PHE:CB	2.32	0.60
1:C:424:LYS:HD3	1:C:431:LYS:HE3	1.83	0.60
1:C:664:ILE:HD11	2:F:18:LEU:HD11	1.84	0.60
1:B:595:ILE:N	1:B:595:ILE:HD12	2.17	0.60
1:B:295:VAL:HG22	1:B:610:MET:HE1	1.84	0.60
1:B:511:LYS:N	1:B:511:LYS:HD2	2.17	0.60
1:B:633:ASN:O	1:B:634:LYS:HB3	2.02	0.60
1:A:657:ILE:HD11	1:A:704:TYR:CE1	2.37	0.60
1:C:630:ARG:NE	2:F:87:GLU:OE2	2.33	0.60
1:B:539:GLU:OE2	2:E:84:GLU:OE1	2.19	0.60
1:B:539:GLU:OE2	2:E:84:GLU:OE2	2.20	0.60
1:C:360:VAL:HG22	1:C:360:VAL:O	2.00	0.60
1:A:605:THR:HA	1:A:610:MET:SD	2.42	0.59
1:A:555:GLN:O	1:A:559:ARG:HG2	2.00	0.59
1:C:752:LEU:O	1:C:755:ARG:N	2.35	0.59
1:C:526:GLN:HB3	2:F:124:MET:HE2	1.83	0.59
2:D:102:ALA:HA	2:D:125:ILE:HG13	1.82	0.59
1:B:715:GLU:HA	1:B:718:ARG:HB3	1.83	0.59
1:B:710:HIS:CB	2:E:127:GLU:HA	2.31	0.59
1:A:302:LEU:HD21	1:A:309:PRO:HG3	1.83	0.59
1:A:781:ASN:ND2	1:A:789:ASN:HA	2.17	0.59
1:C:535:LYS:HD2	1:C:536:TYR:CE1	2.37	0.59
1:A:783:THR:OG1	1:A:783:THR:O	1.93	0.59
1:B:329:ARG:CG	1:B:330:PRO:HD2	2.32	0.59
1:C:369:ASP:OD1	1:C:442:TYR:HE1	1.86	0.59
1:B:327:LEU:HB3	1:B:495:PHE:HB3	1.83	0.59
1:C:550:SER:O	1:C:554:LYS:HB2	2.02	0.59
1:A:539:GLU:CG	2:D:84:GLU:CD	2.71	0.59
1:A:499:PRO:HD3	1:A:552:TRP:CH2	2.37	0.59
2:F:22:ASP:HB2	2:F:26:THR:HB	1.85	0.59
1:C:410:ILE:O	1:C:414:LYS:HB2	2.00	0.59
1:C:344:ALA:O	1:C:488:LEU:HA	2.03	0.59
1:B:749:PHE:C	1:B:751:TYR:H	2.06	0.59
1:A:764:LEU:C	1:A:766:HIS:H	2.04	0.59
1:C:777:TYR:CE1	1:C:780:LEU:HD21	2.37	0.59
1:B:549:LEU:H	1:B:549:LEU:HD12	1.67	0.59
1:B:306:GLY:HA3	1:B:331:VAL:HG13	1.85	0.59
1:A:668:SER:O	1:A:670:ILE:N	2.32	0.59
1:B:502:THR:OG1	1:B:503:GLU:N	2.32	0.58
1:B:534:ILE:O	1:B:538:ILE:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:THR:C	2:D:81:SER:H	2.07	0.58
1:B:520:PRO:O	1:B:521:ASN:HB2	2.03	0.58
1:A:310:GLU:HG3	1:A:340:LYS:HZ2	1.68	0.58
1:A:778:LYS:HB3	1:A:778:LYS:NZ	2.18	0.58
1:B:319:ALA:HB1	1:B:324:THR:O	2.03	0.58
1:C:540:ARG:HD3	1:C:627:TYR:CZ	2.38	0.58
2:F:85:ILE:O	2:F:87:GLU:N	2.36	0.58
1:C:759:GLN:NE2	1:C:762:LEU:HD23	2.18	0.58
1:A:350:VAL:HG21	1:A:488:LEU:HD13	1.86	0.58
1:C:700:TYR:CD1	1:C:727:GLN:HB3	2.39	0.58
1:A:418:ILE:HG22	1:A:419:ILE:HG23	1.85	0.58
1:B:325:TYR:HB2	1:B:498:ALA:HB3	1.84	0.58
1:B:324:THR:CB	1:B:499:PRO:HA	2.28	0.58
1:B:654:ILE:HA	1:B:755:ARG:CG	2.24	0.58
2:D:105:LEU:HD23	2:D:105:LEU:O	2.03	0.58
1:B:327:LEU:HD11	1:B:595:ILE:CG2	2.33	0.58
1:C:732:ILE:HG22	1:C:732:ILE:O	2.03	0.58
2:F:50:ASP:OD1	2:F:51:MET:HG3	2.03	0.58
1:A:661:ALA:HB2	2:D:39:LEU:O	2.04	0.58
2:E:107:HIS:HA	2:E:110:THR:OG1	2.04	0.58
1:A:659:THR:HG23	1:A:662:GLU:H	1.69	0.58
1:B:552:TRP:C	1:B:552:TRP:CD1	2.77	0.58
1:A:792:VAL:O	1:A:796:ILE:HG12	2.04	0.58
2:D:7:GLU:C	2:D:9:ILE:H	2.06	0.58
1:B:366:PHE:HD1	1:B:477:MET:CE	2.15	0.58
1:A:509:PRO:HG2	1:A:512:GLU:HB3	1.86	0.58
2:F:65:PHE:HB2	2:F:66:PRO:HD3	1.85	0.58
2:E:20:ASP:OD1	2:E:27:ILE:HG22	2.04	0.58
1:A:509:PRO:O	1:A:511:LYS:N	2.33	0.57
1:C:496:ALA:HB1	1:C:626:TYR:HE1	1.68	0.57
1:C:740:GLN:O	1:C:741:ILE:O	2.20	0.57
1:A:629:ASN:HB3	1:A:632:TYR:CD2	2.39	0.57
2:F:83:GLU:C	2:F:85:ILE:H	2.07	0.57
1:B:643:ILE:N	1:B:643:ILE:HD12	2.19	0.57
2:F:41:GLN:NE2	2:F:75:LYS:HD2	2.19	0.57
1:B:439:ASN:ND2	1:B:441:VAL:H	2.01	0.57
1:C:505:LYS:NZ	1:C:513:TRP:CD2	2.72	0.57
2:D:55:VAL:HG13	2:D:56:ASP:H	1.70	0.57
1:B:536:TYR:N	1:B:536:TYR:HD2	2.01	0.57
1:B:518:ASN:C	1:B:520:PRO:HD3	2.24	0.57
2:F:117:THR:C	2:F:119:GLU:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LYS:C	1:B:753:LYS:HD3	2.25	0.57
1:A:495:PHE:HA	1:A:580:GLU:HB2	1.86	0.57
2:E:65:PHE:C	2:E:67:GLU:H	2.08	0.57
2:E:93:ASP:HA	2:E:104:GLU:OE2	2.04	0.57
2:F:74:ARG:N	2:F:77:LYS:HB2	2.20	0.57
1:B:439:ASN:HD22	1:B:442:TYR:H	1.51	0.57
1:C:295:VAL:HG22	1:C:603:ILE:HG22	1.87	0.57
2:F:83:GLU:O	2:F:85:ILE:N	2.38	0.57
1:B:329:ARG:NH2	1:B:588:GLU:CB	2.68	0.57
1:A:384:ASN:O	1:A:387:ASN:N	2.37	0.57
1:B:629:ASN:OD1	1:B:631:SER:HB2	2.05	0.57
2:F:143:GLN:C	2:F:145:MET:H	2.08	0.57
1:C:478:ALA:HA	1:C:488:LEU:HD12	1.87	0.57
1:B:495:PHE:O	1:B:581:GLN:HG2	2.05	0.56
1:B:706:ASN:N	2:E:130:ILE:CG2	2.68	0.56
2:E:105:LEU:HD13	2:E:125:ILE:CD1	2.35	0.56
2:E:130:ILE:HG22	2:E:130:ILE:O	2.03	0.56
1:B:368:GLN:HG3	1:B:384:ASN:N	2.20	0.56
1:C:527:LYS:HE3	1:C:531:ASN:HD22	1.69	0.56
1:B:717:LYS:C	1:B:719:LYS:H	2.08	0.56
1:B:294:ASP:HB3	1:B:606:LYS:HZ2	1.69	0.56
1:C:561:ASN:O	1:C:564:VAL:HG22	2.05	0.56
2:E:92:PHE:CZ	2:E:108:VAL:HG11	2.40	0.56
1:B:628:PHE:C	1:B:628:PHE:CD1	2.79	0.56
1:B:342:GLY:HA2	1:B:569:TYR:CD1	2.40	0.56
1:B:310:GLU:O	1:B:314:ALA:HB3	2.06	0.56
1:B:500:SER:O	1:B:503:GLU:HB2	2.05	0.56
2:F:93:ASP:OD1	2:F:99:TYR:O	2.23	0.56
2:E:100:ILE:HB	2:E:136:VAL:HB	1.87	0.56
2:F:120:GLU:O	2:F:124:MET:HG3	2.05	0.56
1:C:346:LYS:HD3	1:C:364:ILE:CD1	2.36	0.56
1:C:774:LYS:C	1:C:775:LEU:HD12	2.25	0.56
1:C:525:LYS:O	1:C:529:VAL:HG23	2.06	0.56
1:B:536:TYR:CD2	1:B:536:TYR:N	2.73	0.56
1:C:797:ILE:HG13	1:C:798:ASP:N	2.20	0.56
1:A:613:ARG:HG2	1:A:613:ARG:NH2	2.19	0.56
1:A:657:ILE:CG2	1:A:756:ILE:HA	2.35	0.56
2:D:87:GLU:O	2:D:91:VAL:HG23	2.05	0.56
1:C:656:THR:O	1:C:755:ARG:HD2	2.05	0.56
1:A:789:ASN:N	1:A:789:ASN:HD22	2.01	0.56
1:B:295:VAL:HG22	1:B:610:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ASP:C	1:C:427:ASP:OD2	2.43	0.56
1:B:386:GLU:HA	1:B:389:LYS:CE	2.36	0.56
1:C:463:THR:CG2	1:C:464:VAL:N	2.69	0.56
1:C:775:LEU:HD12	1:C:775:LEU:N	2.20	0.56
1:B:359:PRO:HG2	1:B:444:PHE:CD2	2.41	0.56
1:B:593:ILE:CG1	1:B:611:THR:HG21	2.35	0.56
1:A:577:HIS:CE1	5:A:289:CMP:N3	2.74	0.56
1:B:730:ASN:O	1:B:733:GLU:N	2.37	0.56
1:B:529:VAL:HG21	2:E:109:MET:SD	2.46	0.56
1:B:621:GLY:O	1:B:622:LYS:HB2	2.06	0.56
1:B:351:HIS:HB2	1:B:386:GLU:HG3	1.86	0.56
1:B:399:GLY:O	1:B:478:ALA:N	2.36	0.56
2:F:16:PHE:H	2:F:16:PHE:HD1	1.53	0.56
1:A:302:LEU:HD23	1:A:303:LYS:N	2.21	0.55
1:B:316:LYS:O	1:B:320:ARG:HB2	2.05	0.55
1:C:540:ARG:NH2	2:F:87:GLU:OE1	2.39	0.55
2:F:27:ILE:HG13	2:F:63:ILE:CD1	2.36	0.55
1:A:346:LYS:HD2	1:A:364:ILE:HD11	1.88	0.55
1:A:541:LYS:HB2	1:A:541:LYS:HZ3	1.69	0.55
1:C:723:PHE:HE2	1:C:727:GLN:NE2	2.04	0.55
1:B:712:PHE:CD2	1:B:716:LYS:HG2	2.38	0.55
1:B:744:GLU:OE1	1:B:744:GLU:HA	2.07	0.55
1:B:463:THR:CG2	1:B:464:VAL:N	2.69	0.55
1:A:540:ARG:HD3	1:A:627:TYR:CZ	2.42	0.55
1:B:628:PHE:CD1	1:B:628:PHE:O	2.59	0.55
1:A:657:ILE:CG2	1:A:756:ILE:HD13	2.36	0.55
1:A:445:ARG:HG3	1:A:471:TRP:CH2	2.41	0.55
2:D:55:VAL:HG13	2:D:56:ASP:N	2.20	0.55
1:C:665:LYS:HG2	2:F:11:GLU:OE2	2.07	0.55
1:C:607:ASN:ND2	1:C:609:GLU:HB2	2.21	0.55
2:F:95:ASP:OD2	2:F:104:GLU:OE1	2.20	0.55
1:A:668:SER:HB2	2:D:11:GLU:HA	1.88	0.55
2:E:97:ASN:OD1	2:E:99:TYR:N	2.34	0.55
1:B:327:LEU:CD1	1:B:595:ILE:HG13	2.37	0.55
1:B:595:ILE:HD13	1:B:603:ILE:HB	1.87	0.55
1:B:530:THR:HG22	2:E:92:PHE:CZ	2.42	0.55
1:C:369:ASP:OD1	1:C:442:TYR:CE1	2.59	0.55
1:C:741:ILE:O	1:C:741:ILE:N	2.39	0.55
1:C:318:ILE:HD11	1:C:563:ALA:HB2	1.89	0.55
2:D:77:LYS:O	2:D:80:ASP:HB2	2.06	0.55
1:B:430:LYS:HB2	1:B:432:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ILE:CD1	1:B:649:ILE:N	2.69	0.55
1:C:695:LYS:C	1:C:697:ILE:H	2.10	0.55
1:A:497:LEU:O	1:A:552:TRP:HH2	1.90	0.55
1:B:514:ASP:O	1:B:517:VAL:HG12	2.07	0.55
2:F:29:THR:OG1	2:F:52:ILE:HG12	2.06	0.55
1:B:533:LEU:O	1:B:533:LEU:HD22	2.07	0.55
1:A:715:GLU:HG3	1:A:716:LYS:N	2.21	0.55
1:A:595:ILE:HB	1:A:603:ILE:HD13	1.89	0.55
1:A:404:LYS:HE2	1:A:452:GLU:CG	2.37	0.55
1:A:697:ILE:HG12	1:A:731:GLU:CB	2.36	0.55
1:B:508:ILE:HA	1:B:536:TYR:CD1	2.42	0.55
1:B:302:LEU:O	1:B:302:LEU:HD13	2.07	0.55
1:A:294:ASP:O	1:A:606:LYS:HD3	2.07	0.54
1:C:776:LEU:HD23	1:C:779:GLN:HE22	1.71	0.54
1:B:741:ILE:CG2	1:B:745:TYR:HB2	2.34	0.54
1:A:719:LYS:CE	1:A:767:GLN:HE21	2.21	0.54
2:F:27:ILE:H	2:F:63:ILE:HB	1.72	0.54
1:A:324:THR:HG22	1:A:499:PRO:HA	1.90	0.54
1:A:492:TYR:CD2	1:A:574:VAL:HG13	2.43	0.54
1:B:526:GLN:CG	1:B:527:LYS:H	2.19	0.54
1:A:663:PHE:HE1	1:A:752:LEU:HD11	1.72	0.54
1:C:481:VAL:HG23	1:C:481:VAL:O	2.07	0.54
1:C:662:GLU:O	1:C:666:ASN:HB2	2.07	0.54
1:B:763:LEU:HD12	1:B:764:LEU:N	2.23	0.54
1:A:781:ASN:HD21	1:A:789:ASN:HA	1.72	0.54
2:F:130:ILE:O	2:F:130:ILE:HG22	2.08	0.54
1:C:695:LYS:C	1:C:697:ILE:N	2.58	0.54
1:A:357:TRP:O	1:A:361:ALA:HB2	2.08	0.54
1:A:470:ASN:ND2	1:A:471:TRP:H	2.06	0.54
1:A:613:ARG:HG2	1:A:613:ARG:HH21	1.73	0.54
1:B:752:LEU:O	1:B:756:ILE:HG13	2.08	0.54
1:A:318:ILE:N	1:A:318:ILE:CD1	2.71	0.54
2:E:20:ASP:OD2	2:E:22:ASP:HB3	2.07	0.54
1:B:561:ASN:C	1:B:563:ALA:N	2.61	0.54
2:D:65:PHE:HB2	2:D:66:PRO:CD	2.38	0.54
2:D:12:PHE:CD1	2:D:39:LEU:HD21	2.43	0.54
2:F:12:PHE:HE1	2:F:39:LEU:HD21	1.73	0.54
1:B:526:GLN:C	1:B:528:GLY:H	2.12	0.54
1:B:381:GLU:HG3	1:B:465:LEU:HD21	1.89	0.54
1:C:664:ILE:HD11	2:F:18:LEU:CD1	2.38	0.54
1:A:530:THR:HG21	2:D:145:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:LEU:HD12	1:B:623:ASP:O	2.08	0.54
1:C:654:ILE:HD12	1:C:654:ILE:N	2.23	0.54
1:A:332:ASN:O	1:A:335:ALA:HB3	2.08	0.54
1:B:717:LYS:CA	1:B:720:ILE:HG12	2.33	0.53
2:D:120:GLU:O	2:D:123:GLU:N	2.33	0.53
1:A:359:PRO:HD3	1:A:419:ILE:HG21	1.90	0.53
2:D:133:ASP:OD1	2:D:135:GLN:HG3	2.08	0.53
1:B:526:GLN:HG3	1:B:527:LYS:H	1.73	0.53
1:A:607:ASN:O	1:A:610:MET:N	2.41	0.53
1:B:338:LEU:HD11	1:B:409:ARG:CZ	2.39	0.53
1:C:526:GLN:NE2	2:F:124:MET:HB3	2.24	0.53
1:A:581:GLN:HA	1:A:581:GLN:OE1	2.07	0.53
1:A:359:PRO:HB2	1:A:405:LEU:HD11	1.91	0.53
1:C:694:VAL:HG23	1:C:695:LYS:N	2.24	0.53
1:B:509:PRO:HD2	1:B:536:TYR:HE1	1.73	0.53
1:B:401:ILE:CG2	1:B:485:LEU:HD23	2.39	0.53
1:B:587:PRO:HD2	1:B:639:ASN:HD21	1.73	0.53
2:E:34:THR:N	2:E:37:ARG:HH21	2.06	0.53
1:C:741:ILE:HG12	1:C:741:ILE:N	2.22	0.53
1:B:316:LYS:C	1:B:318:ILE:H	2.12	0.53
1:B:443:GLU:HG3	1:B:458:LYS:CD	2.36	0.53
1:A:470:ASN:ND2	1:A:471:TRP:N	2.56	0.53
1:B:384:ASN:O	1:B:385:LEU:C	2.47	0.53
1:C:632:TYR:C	1:C:633:ASN:HD22	2.10	0.53
1:B:322:LEU:O	1:B:324:THR:CG2	2.40	0.53
1:B:463:THR:HG22	1:B:464:VAL:N	2.23	0.53
1:B:562:GLU:HA	1:B:565:LYS:CD	2.38	0.53
2:F:117:THR:C	2:F:119:GLU:N	2.62	0.53
1:A:665:LYS:HG2	2:D:11:GLU:CD	2.29	0.53
2:E:20:ASP:C	2:E:22:ASP:H	2.12	0.53
1:A:720:ILE:HD12	1:A:724:ARG:NH1	2.23	0.53
1:A:367:ASP:O	1:A:369:ASP:N	2.42	0.53
1:A:633:ASN:HD21	1:A:645:TRP:H	1.55	0.53
1:A:621:GLY:O	2:D:94:LYS:NZ	2.41	0.53
1:C:650:THR:O	1:C:652:ALA:N	2.42	0.53
1:C:697:ILE:HD11	1:C:731:GLU:O	2.09	0.53
1:A:302:LEU:C	1:A:302:LEU:HD23	2.30	0.53
1:B:345:THR:CG2	1:B:491:ASP:HB3	2.39	0.52
1:B:385:LEU:HA	1:B:388:LYS:HE3	1.92	0.52
1:B:734:ASN:O	1:B:738:SER:HB2	2.09	0.52
1:A:295:VAL:HG21	1:A:603:ILE:CG2	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ARG:CZ	1:A:471:TRP:NE1	2.72	0.52
1:B:372:LYS:O	1:B:374:HIS:N	2.39	0.52
1:B:743:PRO:HA	1:B:746:LYS:HB3	1.92	0.52
2:E:41:GLN:NE2	2:E:75:LYS:HD2	2.24	0.52
1:B:403:LEU:HB2	1:B:476:VAL:CG2	2.39	0.52
1:A:788:ASP:O	1:A:791:GLU:HB2	2.10	0.52
1:A:559:ARG:HH11	1:A:559:ARG:HA	1.74	0.52
1:A:445:ARG:HH22	1:A:456:LYS:HB3	1.73	0.52
1:C:424:LYS:HG2	1:C:425:GLU:N	2.24	0.52
2:F:29:THR:HG21	2:F:52:ILE:HG21	1.91	0.52
1:B:583:ASN:ND2	5:B:290:CMP:O4'	2.43	0.52
1:A:663:PHE:CE1	1:A:752:LEU:HD11	2.45	0.52
1:A:540:ARG:HD3	1:A:627:TYR:OH	2.09	0.52
1:A:529:VAL:HG11	2:D:109:MET:SD	2.49	0.52
1:C:560:LEU:O	1:C:564:VAL:HG13	2.09	0.52
1:B:628:PHE:HD1	1:B:628:PHE:O	1.93	0.52
2:D:118:ASP:N	2:D:118:ASP:OD2	2.42	0.52
1:C:302:LEU:HD21	1:C:309:PRO:HB3	1.92	0.52
1:A:293:ILE:HG21	1:A:610:MET:HG3	1.91	0.52
2:D:41:GLN:HE22	2:D:75:LYS:C	2.13	0.52
1:C:697:ILE:CG1	1:C:731:GLU:HB3	2.40	0.52
1:A:643:ILE:N	1:A:643:ILE:HD12	2.25	0.52
1:B:499:PRO:HG2	1:B:504:ILE:HD11	1.92	0.52
1:B:334:LEU:HD22	1:B:334:LEU:H	1.74	0.52
1:B:481:VAL:O	1:B:484:VAL:HG23	2.10	0.52
1:C:746:LYS:HD3	1:C:746:LYS:O	2.10	0.52
1:B:628:PHE:HD1	1:B:628:PHE:C	2.13	0.52
1:B:328:PHE:CE2	1:B:492:TYR:HB3	2.45	0.52
1:A:660:SER:O	1:A:663:PHE:HB3	2.10	0.52
1:A:629:ASN:HD21	1:A:631:SER:HB2	1.75	0.52
2:D:85:ILE:O	2:D:88:ALA:N	2.41	0.52
1:A:445:ARG:NH2	1:A:471:TRP:CD1	2.77	0.52
1:C:656:THR:HG21	2:F:139:GLU:OE1	2.10	0.52
1:B:583:ASN:C	1:B:629:ASN:HD21	2.13	0.52
1:C:629:ASN:HD22	1:C:631:SER:N	2.05	0.52
1:B:756:ILE:O	1:B:760:VAL:HG13	2.10	0.52
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.91	0.52
2:F:22:ASP:OD2	2:F:26:THR:N	2.43	0.52
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.41	0.51
1:B:450:ASN:N	1:B:450:ASN:ND2	2.51	0.51
1:A:384:ASN:O	1:A:385:LEU:C	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:THR:CG2	2:F:52:ILE:HG21	2.40	0.51
1:A:406:ASP:O	1:A:408:LEU:N	2.43	0.51
1:A:415:GLU:C	1:A:417:GLY:H	2.13	0.51
1:C:757:THR:O	1:C:761:GLN:HB2	2.10	0.51
1:B:502:THR:O	1:B:504:ILE:N	2.42	0.51
2:F:27:ILE:C	2:F:63:ILE:HD12	2.31	0.51
1:C:733:GLU:O	1:C:737:LYS:HE2	2.10	0.51
1:B:360:VAL:O	1:B:361:ALA:C	2.48	0.51
1:C:585:GLU:HB3	1:C:586:PHE:CD1	2.44	0.51
1:B:464:VAL:CG2	1:B:465:LEU:N	2.74	0.51
1:A:658:PRO:O	1:A:701:LEU:HD13	2.10	0.51
1:C:668:SER:OG	1:C:669:SER:N	2.44	0.51
1:C:735:VAL:O	1:C:738:SER:HB3	2.11	0.51
1:B:513:TRP:CZ2	2:E:113:GLY:HA3	2.45	0.51
1:B:335:ALA:HB1	1:B:489:THR:OG1	2.11	0.51
1:A:445:ARG:HH22	1:A:456:LYS:CB	2.24	0.51
2:F:44:THR:HG22	2:F:47:GLU:HG3	1.91	0.51
1:C:329:ARG:O	1:C:330:PRO:O	2.28	0.51
1:B:427:ASP:C	1:B:429:GLY:N	2.64	0.51
1:B:484:VAL:HG12	1:B:485:LEU:H	1.75	0.51
1:B:457:THR:HG21	1:B:468:LYS:HA	1.91	0.51
1:A:639:ASN:ND2	1:A:641:ALA:H	2.09	0.51
1:C:597:ASN:HD21	1:C:601:GLU:HB2	1.76	0.51
1:A:543:ASP:HB2	1:A:554:LYS:HE2	1.91	0.51
1:B:327:LEU:HD13	1:B:595:ILE:HG23	1.91	0.51
1:B:492:TYR:CE2	1:B:574:VAL:HG21	2.45	0.51
1:B:658:PRO:HB3	2:E:39:LEU:O	2.10	0.51
1:B:456:LYS:CB	1:B:471:TRP:H	2.14	0.51
2:F:88:ALA:HA	2:F:91:VAL:HG23	1.92	0.51
1:B:620:THR:HG23	1:B:621:GLY:N	2.26	0.51
1:C:659:THR:HG23	2:F:139:GLU:HG3	1.93	0.51
1:A:481:VAL:CG2	1:A:481:VAL:O	2.57	0.51
1:B:480:ASN:HA	1:B:484:VAL:O	2.10	0.51
1:C:346:LYS:HD2	1:C:350:VAL:O	2.10	0.51
1:B:314:ALA:HA	1:B:317:LYS:HE2	1.93	0.51
1:B:657:ILE:HG23	1:B:658:PRO:N	2.25	0.51
1:B:653:LYS:O	1:B:654:ILE:HG23	2.11	0.51
2:F:121:VAL:C	2:F:123:GLU:N	2.64	0.51
1:C:714:GLN:O	1:C:717:LYS:HB2	2.11	0.51
1:B:470:ASN:O	1:B:471:TRP:O	2.29	0.50
1:A:521:ASN:ND2	1:A:522:SER:N	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:LYS:HA	2:F:18:LEU:HD22	1.93	0.50
2:E:16:PHE:H	2:E:16:PHE:HD1	1.58	0.50
1:C:583:ASN:O	1:C:629:ASN:OD1	2.29	0.50
1:B:494:LEU:O	1:B:579:THR:HA	2.12	0.50
1:B:654:ILE:HD12	1:B:654:ILE:C	2.31	0.50
1:A:773:PHE:HA	1:A:776:LEU:CD1	2.33	0.50
2:E:24:ASP:O	2:E:26:THR:N	2.44	0.50
1:C:736:LEU:CD1	1:C:746:LYS:HE2	2.40	0.50
1:A:549:LEU:HD13	1:A:554:LYS:HG3	1.93	0.50
1:A:421:LYS:HE2	1:A:433:TYR:CG	2.46	0.50
1:A:732:ILE:HD13	1:A:752:LEU:HD13	1.92	0.50
2:D:65:PHE:N	2:D:65:PHE:CD1	2.79	0.50
1:C:523:LEU:HD11	2:F:144:MET:CG	2.41	0.50
1:C:607:ASN:OD1	1:C:610:MET:CB	2.59	0.50
1:A:639:ASN:H	1:A:639:ASN:HD22	1.59	0.50
1:C:508:ILE:HG12	1:C:536:TYR:CD2	2.44	0.50
2:F:44:THR:CG2	2:F:47:GLU:HG3	2.41	0.50
1:C:650:THR:C	1:C:652:ALA:H	2.14	0.50
2:E:65:PHE:O	2:E:67:GLU:N	2.45	0.50
1:A:640:LYS:HB3	1:B:385:LEU:HD12	1.93	0.50
1:B:400:LYS:HA	1:B:476:VAL:O	2.11	0.50
2:D:22:ASP:CG	2:D:26:THR:H	2.14	0.50
1:A:408:LEU:O	1:A:408:LEU:HD23	2.12	0.50
1:C:349:ASN:H	1:C:349:ASN:HD22	1.58	0.50
1:C:695:LYS:HD2	2:F:18:LEU:HB3	1.92	0.50
1:A:636:ALA:HB3	1:A:639:ASN:HD21	1.76	0.50
1:C:711:ILE:HG13	1:C:712:PHE:CD2	2.46	0.50
1:B:338:LEU:HB3	1:B:343:VAL:CG2	2.42	0.50
1:B:372:LYS:C	1:B:374:HIS:H	2.14	0.50
1:A:597:ASN:C	1:A:599:GLU:H	2.15	0.50
1:B:308:VAL:HB	1:B:311:HIS:ND1	2.26	0.50
2:F:22:ASP:OD2	2:F:26:THR:CB	2.60	0.50
1:C:604:LEU:HD23	1:C:604:LEU:O	2.12	0.50
1:C:619:ILE:HG22	1:C:620:THR:N	2.27	0.50
1:C:694:VAL:HG23	1:C:695:LYS:H	1.75	0.50
1:C:777:TYR:O	1:C:780:LEU:HG	2.12	0.50
1:B:626:TYR:CD2	1:B:627:TYR:N	2.80	0.50
1:B:585:GLU:O	1:B:638:GLY:HA3	2.12	0.50
1:C:514:ASP:HA	1:C:517:VAL:CG1	2.40	0.50
1:C:527:LYS:HE3	1:C:531:ASN:ND2	2.27	0.50
2:F:121:VAL:O	2:F:123:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:22:ASP:CB	2:F:26:THR:HB	2.42	0.50
2:F:55:VAL:HG13	2:F:56:ASP:N	2.27	0.50
1:A:741:ILE:HG22	1:A:742:ALA:N	2.27	0.50
1:B:788:ASP:O	1:B:791:GLU:HG2	2.11	0.50
2:E:102:ALA:HB1	2:E:121:VAL:CG1	2.42	0.49
1:B:372:LYS:HG3	1:B:373:LYS:N	2.27	0.49
1:B:504:ILE:N	1:B:504:ILE:HD13	2.27	0.49
1:C:605:THR:CG2	1:C:611:THR:HA	2.36	0.49
1:A:440:GLN:HG2	1:A:440:GLN:O	2.11	0.49
1:B:565:LYS:C	1:B:567:THR:N	2.66	0.49
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.94	0.49
1:B:320:ARG:CG	1:B:598:PRO:O	2.49	0.49
2:D:64:ASP:HB3	2:D:65:PHE:CD1	2.47	0.49
1:A:584:GLU:OE1	1:A:630:ARG:HG3	2.13	0.49
1:A:746:LYS:HD3	1:A:746:LYS:C	2.33	0.49
1:C:390:SER:O	1:C:394:HIS:HB2	2.12	0.49
1:B:310:GLU:O	1:B:314:ALA:CB	2.60	0.49
1:B:508:ILE:HG23	1:B:536:TYR:CD1	2.47	0.49
1:B:748:TYR:O	1:B:751:TYR:HB3	2.13	0.49
1:C:622:LYS:O	1:C:623:ASP:HB2	2.12	0.49
2:E:87:GLU:O	2:E:91:VAL:HG23	2.13	0.49
1:B:307:LEU:HD13	1:B:312:ALA:HB2	1.93	0.49
1:B:722:ILE:HD11	1:B:763:LEU:CD1	2.42	0.49
1:C:495:PHE:HA	1:C:580:GLU:HB2	1.94	0.49
1:C:304:ALA:HB3	1:C:604:LEU:CD1	2.41	0.49
1:B:447:SER:OG	1:B:450:ASN:ND2	2.45	0.49
1:C:305:SER:OG	1:C:306:GLY:N	2.45	0.49
1:A:657:ILE:HG21	1:A:756:ILE:HD13	1.93	0.49
1:A:295:VAL:HG22	1:A:296:LEU:N	2.28	0.49
1:B:714:GLN:NE2	1:B:714:GLN:H	2.09	0.49
1:C:639:ASN:C	1:C:639:ASN:ND2	2.66	0.49
1:A:700:TYR:CD1	1:A:727:GLN:HB3	2.47	0.49
1:B:732:ILE:HG22	1:B:732:ILE:O	2.12	0.49
1:A:794:GLN:O	1:A:797:ILE:HD11	2.12	0.49
1:A:329:ARG:HB3	1:A:330:PRO:CD	2.43	0.49
1:C:643:ILE:HD12	1:C:643:ILE:N	2.28	0.49
1:C:470:ASN:CG	1:C:471:TRP:H	2.16	0.49
1:B:405:LEU:HB3	1:B:410:ILE:HD11	1.93	0.49
1:C:578:GLY:C	5:C:910:CMP:N1	2.66	0.49
1:B:316:LYS:O	1:B:318:ILE:N	2.43	0.49
1:A:629:ASN:ND2	1:A:631:SER:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:THR:O	1:C:766:HIS:ND1	2.46	0.49
1:C:774:LYS:HB3	1:C:775:LEU:HD12	1.95	0.49
1:C:445:ARG:HD3	1:C:471:TRP:CE2	2.48	0.49
1:A:567:THR:HG22	1:A:567:THR:O	2.12	0.49
1:B:726:ILE:HA	1:B:729:TYR:CE2	2.40	0.48
1:B:313:ASP:O	1:B:316:LYS:HG3	2.13	0.48
1:B:712:PHE:HB3	1:B:716:LYS:HG2	1.95	0.48
1:B:450:ASN:N	1:B:450:ASN:HD22	1.94	0.48
1:B:368:GLN:HG3	1:B:383:GLY:C	2.34	0.48
1:B:332:ASN:ND2	1:B:334:LEU:N	2.60	0.48
1:A:574:VAL:CG1	1:A:575:VAL:N	2.76	0.48
1:B:323:ASN:OD1	1:B:500:SER:HB3	2.13	0.48
1:B:748:TYR:CZ	1:B:752:LEU:HD21	2.48	0.48
1:C:408:LEU:O	1:C:408:LEU:HD23	2.12	0.48
1:B:595:ILE:HD12	1:B:603:ILE:O	2.14	0.48
1:B:526:GLN:C	1:B:528:GLY:N	2.66	0.48
1:B:349:ASN:HD21	1:B:398:ILE:HD11	1.76	0.48
1:B:351:HIS:HB2	1:B:386:GLU:CG	2.43	0.48
1:B:387:ASN:O	1:B:388:LYS:C	2.51	0.48
2:D:33:GLY:C	2:D:35:VAL:N	2.66	0.48
1:A:389:LYS:O	1:A:393:GLU:HB2	2.13	0.48
1:C:672:ARG:NE	1:C:672:ARG:HA	2.28	0.48
2:E:129:ASP:OD1	2:E:130:ILE:N	2.46	0.48
1:C:695:LYS:O	1:C:697:ILE:N	2.47	0.48
2:E:33:GLY:O	2:E:37:ARG:N	2.44	0.48
1:C:672:ARG:HE	1:C:672:ARG:HA	1.77	0.48
1:A:657:ILE:HG21	1:A:756:ILE:HA	1.95	0.48
1:B:706:ASN:N	2:E:130:ILE:HG21	2.28	0.48
1:A:294:ASP:O	1:A:610:MET:CE	2.61	0.48
1:C:639:ASN:C	1:C:639:ASN:HD22	2.15	0.48
1:A:357:TRP:C	1:A:361:ALA:HB2	2.34	0.48
1:A:530:THR:O	1:A:533:LEU:HB3	2.14	0.48
1:A:549:LEU:H	1:A:549:LEU:HD12	1.79	0.48
1:A:712:PHE:CE1	1:A:716:LYS:HE2	2.49	0.48
1:B:620:THR:CG2	1:B:621:GLY:N	2.76	0.48
2:D:65:PHE:C	2:D:67:GLU:H	2.16	0.48
1:B:385:LEU:O	1:B:389:LYS:HD3	2.13	0.48
1:B:389:LYS:O	1:B:390:SER:C	2.52	0.48
1:A:320:ARG:HG2	1:A:598:PRO:O	2.13	0.48
1:C:558:ASP:O	1:C:562:GLU:HG3	2.13	0.48
1:A:765:THR:HG22	1:A:765:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:O	1:B:495:PHE:N	2.47	0.48
1:B:654:ILE:O	1:B:759:GLN:HB2	2.14	0.48
1:C:619:ILE:O	1:C:620:THR:C	2.52	0.48
2:E:117:THR:C	2:E:119:GLU:H	2.16	0.48
2:E:16:PHE:CD1	2:E:16:PHE:N	2.82	0.48
1:B:301:ALA:HB1	1:B:604:LEU:HB2	1.96	0.48
1:A:328:PHE:HE1	1:A:596:ILE:HD12	1.79	0.48
1:C:628:PHE:C	1:C:628:PHE:CD1	2.87	0.48
1:C:494:LEU:HB3	1:C:579:THR:HG22	1.95	0.48
1:B:602:PHE:C	1:B:603:ILE:HD13	2.34	0.48
1:A:597:ASN:OD1	1:A:601:GLU:HB2	2.13	0.48
2:F:85:ILE:O	2:F:88:ALA:N	2.33	0.48
1:C:611:THR:O	1:C:611:THR:HG22	2.14	0.48
1:C:562:GLU:O	1:C:565:LYS:N	2.46	0.48
1:A:296:LEU:HB2	1:A:604:LEU:HB3	1.96	0.48
1:A:580:GLU:OE2	1:A:580:GLU:O	2.31	0.47
1:B:373:LYS:HD2	1:B:376:GLN:NE2	2.29	0.47
1:A:463:THR:CG2	1:A:464:VAL:N	2.77	0.47
1:B:615:ILE:HD12	1:B:645:TRP:CH2	2.48	0.47
1:C:788:ASP:O	1:C:792:VAL:HG23	2.14	0.47
1:B:556:MET:O	1:B:560:LEU:HD12	2.14	0.47
1:B:460:GLY:H	1:B:468:LYS:HZ1	1.61	0.47
2:D:33:GLY:O	2:D:37:ARG:HG3	2.14	0.47
1:A:728:ALA:C	1:A:730:ASN:N	2.67	0.47
2:F:70:THR:O	2:F:73:ALA:HB3	2.14	0.47
1:B:513:TRP:HZ2	2:E:113:GLY:HA3	1.79	0.47
1:B:595:ILE:HB	1:B:603:ILE:HB	1.96	0.47
1:A:752:LEU:O	1:A:756:ILE:N	2.41	0.47
2:D:81:SER:C	2:D:83:GLU:H	2.18	0.47
1:C:650:THR:C	1:C:652:ALA:N	2.68	0.47
1:C:317:LYS:HD2	1:C:317:LYS:N	2.29	0.47
2:D:20:ASP:C	2:D:22:ASP:H	2.18	0.47
1:C:580:GLU:C	1:C:582:ASP:H	2.17	0.47
2:F:99:TYR:O	2:F:104:GLU:OE1	2.33	0.47
1:C:659:THR:HG22	1:C:705:TYR:CD1	2.50	0.47
1:C:715:GLU:OE1	1:C:719:LYS:NZ	2.48	0.47
1:B:414:LYS:HZ1	1:B:415:GLU:CD	2.18	0.47
1:A:481:VAL:CG2	1:A:486:LYS:HG3	2.45	0.47
1:A:777:TYR:HA	1:A:780:LEU:HG	1.95	0.47
1:C:700:TYR:CE1	1:C:727:GLN:HB3	2.50	0.47
1:A:706:ASN:O	1:A:708:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ASN:HD21	1:B:442:TYR:N	2.08	0.47
1:A:521:ASN:CG	1:A:522:SER:N	2.68	0.47
1:C:504:ILE:HG23	1:C:536:TYR:O	2.15	0.47
1:A:739:LYS:HG3	1:A:740:GLN:O	2.14	0.47
1:B:705:TYR:HE2	2:E:137:ASN:HD21	1.63	0.47
2:E:75:LYS:C	2:E:77:LYS:N	2.68	0.47
1:B:615:ILE:CD1	1:B:645:TRP:HH2	2.28	0.47
2:F:44:THR:C	2:F:46:ALA:H	2.18	0.47
1:C:711:ILE:HG13	1:C:712:PHE:N	2.30	0.47
2:D:107:HIS:O	2:D:111:ASN:ND2	2.46	0.47
1:C:740:GLN:C	1:C:741:ILE:O	2.52	0.47
1:B:608:TRP:CZ2	1:B:643:ILE:CG2	2.97	0.47
1:C:593:ILE:HG13	1:C:611:THR:HG21	1.95	0.47
1:A:445:ARG:CZ	1:A:471:TRP:CD1	2.98	0.47
1:B:418:ILE:HG22	1:B:419:ILE:HG23	1.96	0.47
2:E:106:ARG:O	2:E:110:THR:HG23	2.15	0.47
1:B:639:ASN:ND2	1:B:641:ALA:HB2	2.30	0.47
1:C:293:ILE:HG22	1:C:613:ARG:HH22	1.80	0.47
1:B:378:LEU:HD23	1:C:377:GLN:NE2	2.30	0.47
1:B:313:ASP:C	1:B:315:PHE:H	2.18	0.47
1:B:527:LYS:HG3	2:E:145:MET:HG3	1.96	0.47
1:C:540:ARG:NH1	1:C:627:TYR:CE1	2.83	0.47
1:A:670:ILE:O	1:A:670:ILE:HG12	2.15	0.47
1:B:761:GLN:HG2	1:B:765:THR:HG23	1.97	0.47
1:A:466:GLY:HA3	1:C:376:GLN:HE22	1.80	0.47
1:C:375:GLY:HA2	1:C:464:VAL:CG2	2.44	0.47
1:C:346:LYS:HD3	1:C:364:ILE:HD11	1.95	0.47
1:A:406:ASP:C	1:A:408:LEU:N	2.68	0.47
1:C:455:TYR:HA	1:C:471:TRP:HZ3	1.80	0.47
1:B:543:ASP:N	1:B:547:GLY:O	2.48	0.47
1:A:615:ILE:HG22	1:A:620:THR:HG23	1.97	0.47
1:B:529:VAL:O	1:B:533:LEU:HB3	2.15	0.47
1:A:470:ASN:HD22	1:A:471:TRP:N	2.12	0.47
1:B:505:LYS:CG	1:B:506:LYS:N	2.78	0.47
2:E:7:GLU:C	2:E:9:ILE:N	2.66	0.47
1:C:639:ASN:N	1:C:639:ASN:HD22	2.13	0.47
2:E:74:ARG:HG2	2:E:74:ARG:HH11	1.80	0.47
1:C:519:THR:OG1	1:C:520:PRO:N	2.48	0.46
1:C:295:VAL:O	1:C:296:LEU:C	2.52	0.46
1:C:295:VAL:CG2	1:C:603:ILE:HG22	2.45	0.46
1:B:539:GLU:CD	2:E:84:GLU:OE2	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:GLN:C	1:C:557:LEU:N	2.68	0.46
2:F:78:ASP:OD1	2:F:79:THR:N	2.48	0.46
1:B:326:ILE:CG2	1:B:596:ILE:HD12	2.42	0.46
1:C:520:PRO:O	1:C:521:ASN:C	2.53	0.46
1:A:711:ILE:HG13	1:A:712:PHE:CD2	2.51	0.46
1:A:597:ASN:ND2	1:A:599:GLU:HB2	2.31	0.46
1:B:553:GLN:O	1:B:557:LEU:N	2.47	0.46
1:B:745:TYR:O	1:B:749:PHE:HD1	1.97	0.46
1:A:761:GLN:HE22	1:A:774:LYS:HA	1.81	0.46
1:B:329:ARG:NH2	1:B:588:GLU:HB3	2.22	0.46
1:C:295:VAL:HG23	1:C:604:LEU:O	2.16	0.46
2:E:81:SER:HA	2:E:84:GLU:HB2	1.98	0.46
1:C:650:THR:HA	1:C:653:LYS:HB2	1.98	0.46
2:F:139:GLU:O	2:F:143:GLN:HG2	2.16	0.46
1:C:765:THR:O	1:C:765:THR:HG22	2.16	0.46
1:B:296:LEU:HB3	1:B:604:LEU:HB3	1.96	0.46
1:B:530:THR:OG1	2:E:145:MET:CE	2.63	0.46
1:B:716:LYS:HG3	1:B:720:ILE:HD13	1.97	0.46
2:F:82:GLU:O	2:F:85:ILE:HB	2.15	0.46
1:B:539:GLU:HG2	2:E:84:GLU:CG	2.42	0.46
1:C:749:PHE:C	1:C:751:TYR:N	2.68	0.46
1:C:714:GLN:NE2	2:F:126:ARG:HG2	2.31	0.46
1:C:669:SER:C	1:C:671:ARG:H	2.19	0.46
2:E:125:ILE:O	2:E:129:ASP:N	2.42	0.46
1:C:635:ILE:O	1:C:636:ALA:C	2.51	0.46
2:E:121:VAL:C	2:E:123:GLU:H	2.18	0.46
1:C:657:ILE:HG23	1:C:756:ILE:CD1	2.45	0.46
1:A:640:LYS:HB3	1:B:385:LEU:CD1	2.46	0.46
1:C:533:LEU:C	1:C:535:LYS:H	2.17	0.46
1:B:478:ALA:HA	1:B:488:LEU:HD22	1.96	0.46
1:A:723:PHE:O	1:A:726:ILE:N	2.48	0.46
1:C:338:LEU:O	1:C:341:SER:HB3	2.16	0.46
1:C:542:PRO:HA	1:C:548:THR:HA	1.98	0.46
1:B:735:VAL:HA	1:B:738:SER:CB	2.46	0.46
1:B:530:THR:HA	1:B:533:LEU:HD12	1.98	0.46
1:A:752:LEU:O	1:A:753:LYS:C	2.53	0.46
2:F:88:ALA:HA	2:F:91:VAL:CG2	2.46	0.46
1:A:633:ASN:ND2	1:A:645:TRP:H	2.14	0.46
2:E:120:GLU:O	2:E:123:GLU:HB3	2.15	0.46
1:C:665:LYS:HG2	2:F:11:GLU:CD	2.36	0.46
2:F:7:GLU:C	2:F:9:ILE:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:LEU:O	2:D:52:ILE:HG22	2.16	0.46
1:A:589:LYS:HG3	1:A:608:TRP:CD2	2.51	0.46
1:B:315:PHE:CE2	1:B:560:LEU:HD23	2.51	0.46
1:C:502:THR:O	1:C:505:LYS:HB3	2.16	0.46
1:B:555:GLN:O	1:B:558:ASP:HB2	2.16	0.46
1:A:443:GLU:O	1:A:455:TYR:HA	2.16	0.46
1:C:302:LEU:HD11	1:C:309:PRO:HA	1.97	0.46
1:B:405:LEU:CB	1:B:410:ILE:HD11	2.45	0.46
1:C:759:GLN:HE22	1:C:762:LEU:HD23	1.80	0.46
1:A:797:ILE:HG13	1:A:798:ASP:N	2.25	0.45
1:B:519:THR:HB	1:B:525:LYS:NZ	2.31	0.45
2:F:12:PHE:CE1	2:F:39:LEU:HD21	2.51	0.45
2:F:9:ILE:HG23	2:F:69:LEU:HD22	1.97	0.45
1:B:766:HIS:HB2	1:B:767:GLN:HE21	1.81	0.45
2:F:33:GLY:O	2:F:37:ARG:N	2.34	0.45
1:B:595:ILE:HD11	1:B:605:THR:HG23	1.98	0.45
1:C:519:THR:CA	1:C:520:PRO:CD	2.94	0.45
1:B:564:VAL:HG11	1:B:574:VAL:HG11	1.97	0.45
1:B:657:ILE:HG23	1:B:658:PRO:CD	2.46	0.45
1:C:533:LEU:C	1:C:535:LYS:N	2.69	0.45
1:C:527:LYS:HD3	1:C:527:LYS:O	2.16	0.45
1:C:349:ASN:N	1:C:349:ASN:HD22	2.14	0.45
1:A:439:ASN:HD22	1:A:440:GLN:H	1.64	0.45
1:C:778:LYS:HD2	1:C:782:PHE:HZ	1.81	0.45
2:F:117:THR:O	2:F:119:GLU:N	2.49	0.45
1:B:306:GLY:C	1:B:331:VAL:HG13	2.36	0.45
2:F:56:ASP:O	2:F:57:ALA:HB2	2.16	0.45
1:B:793:PHE:O	1:B:796:ILE:HG12	2.17	0.45
2:D:117:THR:C	2:D:119:GLU:H	2.19	0.45
1:B:327:LEU:N	1:B:327:LEU:CD2	2.77	0.45
2:E:92:PHE:CD2	2:E:108:VAL:HG21	2.52	0.45
1:B:748:TYR:O	1:B:752:LEU:HG	2.17	0.45
1:B:607:ASN:O	1:B:610:MET:N	2.50	0.45
1:B:447:SER:OG	1:B:449:GLU:HB2	2.17	0.45
1:C:597:ASN:ND2	1:C:601:GLU:HB2	2.31	0.45
1:C:795:LYS:O	1:C:797:ILE:N	2.49	0.45
1:C:370:LEU:HD11	1:C:455:TYR:CE1	2.52	0.45
1:C:421:LYS:HE2	1:C:433:TYR:CB	2.46	0.45
2:F:10:ALA:O	2:F:13:LYS:HB3	2.17	0.45
1:B:503:GLU:C	1:B:504:ILE:HD13	2.37	0.45
1:B:561:ASN:CG	1:B:573:ASP:HB3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LYS:HE2	1:A:767:GLN:NE2	2.31	0.45
1:B:338:LEU:HA	1:B:341:SER:OG	2.16	0.45
1:C:778:LYS:HB3	1:C:778:LYS:HZ3	1.82	0.45
2:D:101:SER:H	2:D:104:GLU:HB2	1.80	0.45
1:B:628:PHE:CD2	1:B:645:TRP:CD1	3.05	0.45
1:B:639:ASN:H	1:B:639:ASN:HD22	1.64	0.45
2:F:87:GLU:O	2:F:91:VAL:HG23	2.17	0.45
1:B:509:PRO:O	1:B:511:LYS:N	2.44	0.45
1:C:641:ALA:HB1	1:C:643:ILE:CD1	2.47	0.45
1:A:661:ALA:HB1	1:A:665:LYS:HZ3	1.82	0.45
2:F:55:VAL:HG13	2:F:56:ASP:H	1.82	0.45
1:A:439:ASN:ND2	1:A:440:GLN:H	2.15	0.45
1:C:351:HIS:CE1	5:C:910:CMP:O3'	2.69	0.45
1:B:561:ASN:C	1:B:563:ALA:H	2.19	0.45
1:B:643:ILE:HD12	1:B:643:ILE:H	1.82	0.45
1:C:735:VAL:HG11	1:C:749:PHE:HE1	1.82	0.45
1:A:736:LEU:HD21	1:A:749:PHE:CB	2.44	0.45
1:A:789:ASN:ND2	1:A:789:ASN:N	2.65	0.45
1:A:537:GLY:C	1:A:538:ILE:HG13	2.30	0.45
1:C:619:ILE:O	1:C:622:LYS:N	2.48	0.45
2:E:103:ALA:O	2:E:106:ARG:HB3	2.17	0.45
1:A:533:LEU:O	1:A:537:GLY:HA3	2.17	0.45
1:B:794:GLN:OE1	1:B:794:GLN:N	2.49	0.45
1:B:605:THR:HG21	1:B:611:THR:CG2	2.43	0.45
1:A:719:LYS:O	1:A:722:ILE:N	2.50	0.45
1:A:338:LEU:O	1:A:341:SER:HB3	2.17	0.45
1:C:427:ASP:OD2	1:C:428:ASN:N	2.50	0.45
1:B:409:ARG:NH1	1:B:412:GLU:OE2	2.50	0.45
2:D:101:SER:O	2:D:102:ALA:C	2.55	0.45
2:E:111:ASN:C	2:E:113:GLY:H	2.20	0.45
1:B:413:LEU:HA	1:B:416:ASN:HB2	1.99	0.45
1:B:607:ASN:O	1:B:608:TRP:C	2.55	0.45
1:B:389:LYS:O	1:B:392:THR:N	2.50	0.45
2:E:20:ASP:OD1	2:E:27:ILE:HA	2.17	0.45
1:C:346:LYS:HB2	1:C:350:VAL:HB	1.98	0.45
1:A:723:PHE:C	1:A:725:GLY:N	2.70	0.45
1:B:766:HIS:CD2	1:B:766:HIS:N	2.85	0.45
1:C:741:ILE:HG22	1:C:742:ALA:N	2.29	0.44
1:A:657:ILE:HG22	1:A:756:ILE:HA	1.98	0.44
1:A:445:ARG:HH22	1:A:456:LYS:CG	2.30	0.44
1:C:315:PHE:O	1:C:316:LYS:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:H	1:C:307:LEU:HD12	1.82	0.44
1:B:557:LEU:HA	1:B:560:LEU:HD12	1.99	0.44
1:B:704:TYR:OH	2:E:131:ASP:HB2	2.17	0.44
1:B:746:LYS:NZ	1:B:750:GLN:NE2	2.66	0.44
1:A:735:VAL:HG11	1:A:749:PHE:HE1	1.81	0.44
2:D:52:ILE:HG23	2:D:53:ASN:N	2.31	0.44
1:B:722:ILE:HD11	1:B:763:LEU:HD11	1.99	0.44
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.98	0.44
2:D:75:LYS:O	2:D:79:THR:HG22	2.17	0.44
1:B:377:GLN:HA	1:B:464:VAL:HG21	1.98	0.44
1:B:649:ILE:C	1:B:651:LYS:N	2.69	0.44
1:B:488:LEU:HD23	1:B:488:LEU:H	1.83	0.44
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.81	0.44
1:B:633:ASN:O	1:B:634:LYS:CB	2.65	0.44
1:B:328:PHE:CZ	1:B:494:LEU:HD21	2.53	0.44
2:F:85:ILE:HG22	2:F:86:ARG:H	1.77	0.44
2:D:65:PHE:CB	2:D:66:PRO:HD3	2.42	0.44
1:B:464:VAL:C	1:B:466:GLY:H	2.21	0.44
1:B:306:GLY:CA	1:B:331:VAL:HG13	2.47	0.44
1:A:709:ASN:C	1:A:711:ILE:H	2.21	0.44
1:A:764:LEU:HD13	1:A:773:PHE:CG	2.53	0.44
1:B:447:SER:C	1:B:449:GLU:N	2.70	0.44
1:C:752:LEU:O	1:C:753:LYS:C	2.55	0.44
1:C:758:ASN:O	1:C:762:LEU:HB2	2.17	0.44
1:B:634:LYS:HB3	1:B:634:LYS:HE2	1.85	0.44
1:B:704:TYR:CE1	1:B:721:SER:HB2	2.53	0.44
2:F:83:GLU:O	2:F:84:GLU:C	2.56	0.44
1:B:406:ASP:C	1:B:408:LEU:H	2.20	0.44
1:A:445:ARG:CD	1:A:471:TRP:CZ2	2.98	0.44
1:C:597:ASN:OD1	1:C:597:ASN:C	2.54	0.44
1:C:411:GLU:OE1	1:C:414:LYS:HD3	2.18	0.44
2:E:20:ASP:O	2:E:22:ASP:N	2.51	0.44
2:E:12:PHE:HB2	2:E:69:LEU:CD2	2.48	0.44
1:B:595:ILE:HD13	1:B:603:ILE:CG2	2.48	0.44
1:C:315:PHE:CE2	1:C:560:LEU:HG	2.52	0.44
1:C:526:GLN:HB3	2:F:124:MET:HE1	1.99	0.44
1:A:367:ASP:C	1:A:369:ASP:H	2.20	0.44
1:A:478:ALA:CB	1:A:485:LEU:HG	2.48	0.44
1:B:783:THR:O	1:B:783:THR:HG22	2.18	0.44
1:A:751:TYR:O	1:A:752:LEU:C	2.54	0.44
1:C:540:ARG:NH1	1:C:582:ASP:OD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:GLN:C	2:F:145:MET:N	2.71	0.44
2:F:14:GLU:OE1	2:F:14:GLU:HA	2.18	0.44
1:B:509:PRO:C	1:B:511:LYS:H	2.20	0.44
1:A:556:MET:HG3	1:A:560:LEU:CD1	2.47	0.44
1:C:499:PRO:HG3	1:C:504:ILE:HD11	1.99	0.44
1:A:450:ASN:OD1	1:A:452:GLU:HG3	2.17	0.44
1:C:747:ASN:ND2	1:C:747:ASN:O	2.51	0.44
1:B:630:ARG:NH2	2:E:87:GLU:OE2	2.48	0.44
1:B:729:TYR:O	1:B:730:ASN:CA	2.64	0.44
1:C:629:ASN:HB3	1:C:632:TYR:CE2	2.52	0.44
1:B:597:ASN:OD1	1:B:601:GLU:HG2	2.18	0.44
1:B:530:THR:O	1:B:534:ILE:N	2.50	0.44
1:B:406:ASP:C	1:B:408:LEU:N	2.70	0.44
2:F:97:ASN:OD1	2:F:99:TYR:O	2.36	0.44
2:D:14:GLU:OE1	2:D:14:GLU:HA	2.18	0.44
2:E:137:ASN:OD1	2:E:139:GLU:HB2	2.18	0.44
2:D:6:GLU:O	2:D:9:ILE:HB	2.18	0.44
1:A:550:SER:O	1:A:554:LYS:HG3	2.17	0.44
1:C:731:GLU:O	1:C:735:VAL:HG23	2.18	0.43
1:A:635:ILE:HD11	1:B:388:LYS:HB3	2.00	0.43
1:A:665:LYS:O	1:A:668:SER:HB3	2.18	0.43
1:C:321:GLU:HG2	1:C:322:LEU:HD23	2.00	0.43
2:E:89:PHE:CE1	2:E:100:ILE:HG13	2.53	0.43
1:C:789:ASN:ND2	1:C:789:ASN:N	2.64	0.43
2:E:137:ASN:O	2:E:138:TYR:C	2.57	0.43
2:F:20:ASP:CG	2:F:22:ASP:OD1	2.56	0.43
1:C:339:ILE:O	1:C:342:GLY:N	2.49	0.43
1:C:434:LEU:O	1:C:435:LEU:HD23	2.18	0.43
1:B:655:ASN:OD1	1:B:755:ARG:NH1	2.52	0.43
1:C:537:GLY:HA2	1:C:552:TRP:NE1	2.34	0.43
2:D:83:GLU:O	2:D:87:GLU:HG3	2.18	0.43
1:A:485:LEU:HA	1:A:485:LEU:HD12	1.81	0.43
1:A:316:LYS:HE2	1:A:602:PHE:CZ	2.53	0.43
1:A:577:HIS:O	1:A:578:GLY:O	2.36	0.43
1:C:520:PRO:C	1:C:521:ASN:C	2.76	0.43
1:B:508:ILE:HA	1:B:536:TYR:CE1	2.53	0.43
1:B:398:ILE:HD13	1:B:398:ILE:HA	1.82	0.43
1:A:377:GLN:HA	1:A:464:VAL:HG11	2.00	0.43
1:A:431:LYS:HE3	1:A:448:ASP:OD1	2.19	0.43
1:A:413:LEU:HD13	1:A:419:ILE:HG12	2.01	0.43
1:C:298:GLY:HA2	1:C:602:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:ASN:HD22	1:C:655:ASN:N	2.15	0.43
1:B:606:LYS:O	1:B:607:ASN:HB3	2.19	0.43
1:B:375:GLY:HA2	1:B:464:VAL:CG1	2.49	0.43
2:E:117:THR:O	2:E:119:GLU:N	2.52	0.43
1:A:739:LYS:HD2	1:A:740:GLN:H	1.84	0.43
1:C:463:THR:HG22	1:C:465:LEU:N	2.33	0.43
1:C:348:LEU:HD23	1:C:348:LEU:HA	1.86	0.43
1:B:500:SER:HA	1:B:624:TYR:HD1	1.74	0.43
1:A:714:GLN:HE22	1:A:717:LYS:NZ	2.15	0.43
1:A:761:GLN:NE2	1:A:773:PHE:CE2	2.87	0.43
1:B:505:LYS:C	1:B:507:GLN:N	2.71	0.43
2:D:120:GLU:O	2:D:121:VAL:C	2.56	0.43
1:B:549:LEU:HD12	1:B:549:LEU:N	2.29	0.43
1:A:415:GLU:C	1:A:417:GLY:N	2.70	0.43
1:C:479:LYS:CG	1:C:480:ASN:H	2.32	0.43
1:B:630:ARG:NE	2:E:87:GLU:OE2	2.48	0.43
1:B:559:ARG:O	1:B:563:ALA:HB2	2.18	0.43
1:B:655:ASN:HB2	1:B:656:THR:H	1.52	0.43
1:A:632:TYR:C	1:A:634:LYS:H	2.21	0.43
1:A:582:ASP:CG	1:A:627:TYR:HH	2.22	0.43
1:B:391:ILE:HA	1:B:391:ILE:HD13	1.75	0.43
1:C:527:LYS:O	1:C:531:ASN:HB2	2.18	0.43
1:A:672:ARG:HA	1:A:672:ARG:NE	2.33	0.43
2:F:22:ASP:OD2	2:F:26:THR:HB	2.19	0.43
2:F:71:MET:C	2:F:73:ALA:N	2.70	0.43
1:B:584:GLU:OE1	1:B:630:ARG:HD2	2.19	0.43
1:B:595:ILE:HD13	1:B:603:ILE:CB	2.48	0.43
1:A:607:ASN:O	1:A:610:MET:HB3	2.19	0.43
1:A:445:ARG:NH2	1:A:456:LYS:HB3	2.33	0.43
1:B:363:TYR:O	1:B:365:PRO:HD3	2.19	0.43
1:B:758:ASN:O	1:B:762:LEU:HB2	2.19	0.43
1:B:453:VAL:HG12	1:B:454:GLN:N	2.33	0.43
1:A:764:LEU:C	1:A:766:HIS:N	2.72	0.43
2:E:105:LEU:HD13	2:E:125:ILE:HD13	2.00	0.43
1:C:557:LEU:O	1:C:560:LEU:N	2.52	0.43
2:D:121:VAL:O	2:D:125:ILE:HG12	2.18	0.43
1:B:480:ASN:CA	1:B:485:LEU:HD12	2.48	0.43
1:B:626:TYR:CD2	1:B:626:TYR:C	2.92	0.43
1:A:297:LYS:HA	1:A:602:PHE:O	2.19	0.43
1:C:741:ILE:H	1:C:741:ILE:CG1	2.27	0.43
1:B:328:PHE:HD2	1:B:493:ASP:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:GLN:O	1:B:528:GLY:N	2.52	0.43
1:B:332:ASN:C	1:B:332:ASN:ND2	2.70	0.43
1:C:781:ASN:O	1:C:782:PHE:C	2.57	0.43
1:B:639:ASN:O	1:B:641:ALA:N	2.51	0.43
1:A:615:ILE:HG22	1:A:620:THR:CG2	2.49	0.43
1:A:787:THR:O	1:A:787:THR:HG22	2.18	0.43
1:B:327:LEU:HA	1:B:327:LEU:HD13	1.79	0.42
1:A:764:LEU:HD13	1:A:773:PHE:HB3	2.00	0.42
1:B:743:PRO:O	1:B:747:ASN:HB3	2.19	0.42
1:C:462:ILE:HD11	1:C:466:GLY:CA	2.48	0.42
1:B:359:PRO:HG2	1:B:444:PHE:CG	2.54	0.42
2:F:16:PHE:CD1	2:F:16:PHE:N	2.86	0.42
1:A:406:ASP:C	1:A:408:LEU:H	2.22	0.42
1:C:434:LEU:HD12	1:C:434:LEU:N	2.33	0.42
1:B:731:GLU:C	1:B:733:GLU:H	2.23	0.42
2:E:92:PHE:HA	2:E:108:VAL:HG21	2.01	0.42
1:A:660:SER:O	1:A:663:PHE:N	2.51	0.42
1:A:318:ILE:H	1:A:318:ILE:CD1	2.33	0.42
1:B:384:ASN:O	1:B:387:ASN:N	2.44	0.42
1:C:776:LEU:N	1:C:776:LEU:HD12	2.35	0.42
1:B:639:ASN:HD22	1:B:639:ASN:N	2.17	0.42
1:C:470:ASN:CG	1:C:471:TRP:N	2.72	0.42
1:C:479:LYS:CG	1:C:480:ASN:N	2.82	0.42
1:B:346:LYS:NZ	1:B:352:GLY:O	2.52	0.42
1:B:751:TYR:O	1:B:755:ARG:N	2.50	0.42
1:A:632:TYR:O	1:A:633:ASN:HB2	2.19	0.42
1:B:446:ILE:HG13	1:B:451:ASN:O	2.18	0.42
1:C:315:PHE:O	1:C:317:LYS:N	2.52	0.42
1:A:639:ASN:HD22	1:A:639:ASN:N	2.15	0.42
1:A:437:SER:C	1:A:439:ASN:H	2.21	0.42
1:B:745:TYR:O	1:B:749:PHE:CD1	2.72	0.42
1:A:712:PHE:O	1:A:717:LYS:HE3	2.19	0.42
1:B:589:LYS:HB2	1:B:643:ILE:HG12	2.00	0.42
1:C:751:TYR:O	1:C:752:LEU:C	2.57	0.42
2:F:123:GLU:C	2:F:125:ILE:N	2.72	0.42
1:C:339:ILE:HD11	1:C:490:ALA:O	2.20	0.42
1:B:748:TYR:CE2	1:B:752:LEU:HD11	2.55	0.42
1:A:766:HIS:CB	1:A:767:GLN:OE1	2.66	0.42
1:B:345:THR:OG1	1:B:491:ASP:HA	2.19	0.42
1:C:749:PHE:C	1:C:751:TYR:H	2.22	0.42
1:A:516:VAL:O	1:A:525:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:HD3	6:A:893:POP:P1	2.58	0.42
1:C:349:ASN:ND2	1:C:349:ASN:H	2.16	0.42
1:A:615:ILE:O	1:A:620:THR:HG23	2.19	0.42
1:A:411:GLU:O	1:A:414:LYS:N	2.53	0.42
1:B:366:PHE:CD1	1:B:477:MET:CE	3.00	0.42
1:A:329:ARG:HB3	1:A:329:ARG:HE	1.61	0.42
1:C:776:LEU:H	1:C:776:LEU:HD12	1.85	0.42
1:A:670:ILE:HA	1:A:672:ARG:NH1	2.33	0.42
1:C:723:PHE:HB2	1:C:793:PHE:CD2	2.54	0.42
1:B:639:ASN:HD21	1:B:641:ALA:CB	2.33	0.42
1:C:307:LEU:N	1:C:307:LEU:HD12	2.35	0.42
1:C:332:ASN:HD22	1:C:333:LYS:N	2.17	0.42
1:B:722:ILE:HG23	1:B:760:VAL:HB	2.00	0.42
1:C:619:ILE:O	1:C:621:GLY:N	2.53	0.42
1:C:666:ASN:C	1:C:666:ASN:HD22	2.22	0.42
1:C:479:LYS:HG2	1:C:480:ASN:N	2.34	0.42
1:C:385:LEU:O	1:C:389:LYS:HG3	2.20	0.42
2:D:137:ASN:OD1	2:D:137:ASN:C	2.58	0.42
2:D:5:THR:OG1	2:D:8:GLN:HB2	2.19	0.42
1:B:722:ILE:CG1	1:B:763:LEU:HD11	2.50	0.42
1:A:719:LYS:CE	1:A:767:GLN:NE2	2.82	0.42
1:A:752:LEU:HA	1:A:752:LEU:HD23	1.89	0.42
2:F:92:PHE:O	2:F:104:GLU:HB3	2.19	0.42
1:C:375:GLY:HA2	1:C:464:VAL:HG22	2.01	0.42
1:C:347:GLY:C	1:C:349:ASN:H	2.23	0.42
1:A:723:PHE:O	1:A:725:GLY:N	2.53	0.42
1:A:745:TYR:O	1:A:748:TYR:HB3	2.20	0.42
1:B:370:LEU:HA	1:B:370:LEU:HD23	1.77	0.42
1:C:632:TYR:HA	1:C:632:TYR:HD2	1.57	0.42
1:B:555:GLN:O	1:B:558:ASP:N	2.46	0.42
2:D:65:PHE:C	2:D:67:GLU:N	2.72	0.42
1:C:551:ASN:C	1:C:553:GLN:N	2.71	0.42
1:A:639:ASN:H	1:A:639:ASN:ND2	2.18	0.42
2:E:139:GLU:O	2:E:142:VAL:HB	2.20	0.42
1:C:384:ASN:O	1:C:385:LEU:C	2.58	0.42
1:A:696:LYS:HG2	1:A:696:LYS:O	2.19	0.42
1:A:697:ILE:CG1	1:A:731:GLU:HB3	2.38	0.42
2:D:81:SER:O	2:D:82:GLU:HB3	2.20	0.42
1:A:791:GLU:O	1:A:794:GLN:HB2	2.20	0.42
2:D:20:ASP:OD1	2:D:22:ASP:OD1	2.38	0.42
1:B:586:PHE:N	1:B:587:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:VAL:CG1	1:B:454:GLN:N	2.83	0.42
2:D:68:PHE:C	2:D:70:THR:N	2.73	0.42
1:A:445:ARG:O	1:A:453:VAL:HA	2.19	0.41
1:C:657:ILE:HG12	1:C:756:ILE:HD13	2.02	0.41
1:C:513:TRP:CZ2	2:F:114:GLU:HB2	2.55	0.41
1:B:509:PRO:HD2	1:B:536:TYR:CE1	2.52	0.41
1:B:416:ASN:HD22	1:B:416:ASN:HA	1.62	0.41
1:A:484:VAL:HG12	1:A:485:LEU:N	2.35	0.41
1:A:411:GLU:OE2	1:A:414:LYS:HE2	2.19	0.41
2:E:6:GLU:O	2:E:10:ALA:N	2.53	0.41
1:B:581:GLN:O	1:B:629:ASN:HA	2.20	0.41
1:B:720:ILE:HG13	1:B:721:SER:N	2.34	0.41
1:A:470:ASN:O	1:A:471:TRP:C	2.57	0.41
1:A:780:LEU:HD12	1:A:780:LEU:C	2.41	0.41
2:D:68:PHE:C	2:D:70:THR:H	2.23	0.41
1:B:561:ASN:OD1	1:B:573:ASP:HB3	2.20	0.41
1:A:722:ILE:HD13	1:A:764:LEU:CG	2.46	0.41
1:B:706:ASN:H	2:E:130:ILE:CG2	2.33	0.41
1:B:744:GLU:C	1:B:746:LYS:N	2.72	0.41
1:A:349:ASN:N	1:A:349:ASN:ND2	2.45	0.41
1:A:539:GLU:CG	2:D:84:GLU:OE1	2.66	0.41
1:B:651:LYS:HG2	1:B:652:ALA:N	2.36	0.41
1:B:539:GLU:CG	2:E:84:GLU:CD	2.88	0.41
1:A:310:GLU:CG	1:A:340:LYS:HZ1	2.34	0.41
2:D:131:ASP:N	2:D:131:ASP:OD1	2.52	0.41
1:B:639:ASN:ND2	1:B:641:ALA:CB	2.83	0.41
1:A:406:ASP:O	1:A:409:ARG:N	2.51	0.41
2:D:33:GLY:O	2:D:35:VAL:N	2.54	0.41
2:D:111:ASN:C	2:D:113:GLY:N	2.73	0.41
2:D:117:THR:C	2:D:119:GLU:N	2.74	0.41
2:D:29:THR:HG22	2:D:29:THR:O	2.20	0.41
1:C:469:PHE:HB2	1:C:472:ARG:HH21	1.85	0.41
1:B:722:ILE:HG12	1:B:763:LEU:HD11	2.03	0.41
1:A:722:ILE:CD1	1:A:764:LEU:HG	2.48	0.41
1:B:450:ASN:O	1:B:451:ASN:HB2	2.20	0.41
2:E:24:ASP:O	2:E:25:GLY:C	2.58	0.41
1:A:541:LYS:CB	1:A:541:LYS:HZ3	2.32	0.41
1:A:728:ALA:C	1:A:730:ASN:H	2.22	0.41
2:F:89:PHE:CE1	2:F:100:ILE:HG13	2.56	0.41
1:B:312:ALA:O	1:B:315:PHE:N	2.50	0.41
1:B:316:LYS:C	1:B:318:ILE:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ASN:O	1:A:711:ILE:N	2.54	0.41
1:A:338:LEU:O	1:A:343:VAL:HG23	2.20	0.41
1:A:541:LYS:CB	1:A:541:LYS:NZ	2.78	0.41
1:A:635:ILE:O	1:A:636:ALA:C	2.59	0.41
2:D:101:SER:O	2:D:104:GLU:HB2	2.20	0.41
1:C:430:LYS:HB2	1:C:432:TYR:CE1	2.56	0.41
1:A:659:THR:HG22	1:A:662:GLU:HB2	2.02	0.41
2:D:80:ASP:O	2:D:80:ASP:OD1	2.38	0.41
1:A:332:ASN:HD22	1:A:332:ASN:C	2.24	0.41
2:D:131:ASP:OD2	2:D:133:ASP:OD2	2.38	0.41
1:B:630:ARG:O	1:B:634:LYS:HD3	2.21	0.41
1:B:657:ILE:CB	1:B:658:PRO:HD2	2.50	0.41
1:B:722:ILE:H	1:B:722:ILE:HG13	1.71	0.41
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.51	0.41
1:B:348:LEU:O	1:B:348:LEU:CD2	2.64	0.41
1:A:540:ARG:NH1	1:A:627:TYR:CZ	2.88	0.41
2:F:143:GLN:O	2:F:145:MET:N	2.53	0.41
2:F:144:MET:SD	2:F:145:MET:HE2	2.60	0.41
1:C:313:ASP:O	1:C:316:LYS:CB	2.65	0.41
2:F:48:LEU:O	2:F:52:ILE:HG22	2.21	0.41
1:B:328:PHE:CD2	1:B:494:LEU:HD23	2.56	0.41
1:B:703:ASP:O	1:B:704:TYR:C	2.58	0.41
2:F:52:ILE:HG23	2:F:53:ASN:N	2.35	0.41
1:A:733:GLU:OE2	1:A:733:GLU:HA	2.20	0.41
2:E:65:PHE:C	2:E:67:GLU:N	2.72	0.41
1:B:511:LYS:N	1:B:511:LYS:CD	2.84	0.41
1:A:497:LEU:CD1	1:A:556:MET:HG2	2.50	0.41
1:C:508:ILE:HG23	1:C:536:TYR:CE2	2.55	0.41
1:C:508:ILE:HD13	1:C:532:LEU:HD13	2.02	0.41
1:A:740:GLN:N	1:A:740:GLN:CD	2.74	0.41
1:A:411:GLU:O	1:A:412:GLU:C	2.58	0.41
2:D:16:PHE:CD1	2:D:16:PHE:N	2.89	0.41
1:B:595:ILE:H	1:B:595:ILE:HD12	1.85	0.41
1:A:629:ASN:HB3	1:A:632:TYR:CE2	2.56	0.41
2:D:65:PHE:O	2:D:67:GLU:N	2.54	0.41
2:D:85:ILE:O	2:D:87:GLU:N	2.53	0.41
2:D:85:ILE:C	2:D:87:GLU:H	2.25	0.41
1:C:658:PRO:HG3	1:C:752:LEU:HD22	2.03	0.41
1:C:315:PHE:O	1:C:318:ILE:N	2.54	0.41
1:B:343:VAL:HG12	1:B:344:ALA:N	2.35	0.41
1:B:385:LEU:O	1:B:388:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:O	1:A:323:ASN:C	2.58	0.41
1:C:504:ILE:O	1:C:507:GLN:N	2.44	0.41
2:D:100:ILE:HA	2:D:104:GLU:OE1	2.20	0.41
1:A:443:GLU:HG3	1:A:458:LYS:CG	2.48	0.41
1:B:325:TYR:CG	1:B:619:ILE:HD11	2.55	0.41
1:C:666:ASN:O	1:C:670:ILE:HB	2.21	0.41
1:A:549:LEU:HD12	1:A:549:LEU:N	2.36	0.41
2:D:70:THR:O	2:D:73:ALA:HB3	2.21	0.41
2:D:136:VAL:HG13	2:D:140:GLU:CB	2.50	0.41
1:C:559:ARG:HA	1:C:559:ARG:HH11	1.85	0.41
1:B:731:GLU:HG3	1:B:732:ILE:N	2.35	0.41
1:C:555:GLN:O	1:C:557:LEU:N	2.54	0.41
1:A:640:LYS:HA	1:A:640:LYS:HD3	1.94	0.41
1:A:534:ILE:HA	1:A:538:ILE:HD12	2.03	0.41
1:A:333:LYS:C	1:A:335:ALA:H	2.24	0.41
1:A:699:GLY:C	1:A:701:LEU:H	2.24	0.41
1:B:788:ASP:C	1:B:790:PHE:H	2.25	0.41
1:C:455:TYR:HA	1:C:471:TRP:CZ3	2.56	0.41
2:E:18:LEU:HA	2:E:18:LEU:HD23	1.93	0.41
1:A:507:GLN:HE21	1:A:507:GLN:HB2	1.69	0.41
2:E:85:ILE:O	2:E:88:ALA:N	2.50	0.40
1:B:655:ASN:HA	1:B:759:GLN:HE22	1.86	0.40
2:F:81:SER:C	2:F:83:GLU:N	2.73	0.40
1:A:593:ILE:CG1	1:A:611:THR:HG21	2.49	0.40
1:C:295:VAL:HG23	1:C:604:LEU:C	2.42	0.40
1:C:514:ASP:O	1:C:518:ASN:N	2.46	0.40
1:C:755:ARG:O	1:C:758:ASN:N	2.54	0.40
1:C:776:LEU:H	1:C:776:LEU:CD1	2.35	0.40
1:A:777:TYR:HA	1:A:780:LEU:CD2	2.52	0.40
1:A:777:TYR:HD1	1:A:780:LEU:HD11	1.84	0.40
2:D:12:PHE:CE1	2:D:39:LEU:HD21	2.56	0.40
1:A:720:ILE:HG13	1:A:721:SER:N	2.35	0.40
1:A:414:LYS:HG3	1:A:420:LEU:HD23	2.03	0.40
1:C:378:LEU:HA	1:C:378:LEU:HD12	1.77	0.40
1:B:561:ASN:O	1:B:564:VAL:N	2.50	0.40
1:A:329:ARG:HD2	1:A:580:GLU:CG	2.46	0.40
1:B:649:ILE:H	1:B:649:ILE:CD1	2.32	0.40
1:B:380:VAL:HG12	1:B:384:ASN:HD22	1.86	0.40
2:F:107:HIS:O	2:F:109:MET:N	2.54	0.40
1:A:335:ALA:O	1:A:339:ILE:HG13	2.19	0.40
1:B:558:ASP:O	1:B:559:ARG:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:LEU:HD13	1:B:534:ILE:N	2.36	0.40
1:B:749:PHE:C	1:B:751:TYR:N	2.73	0.40
1:A:425:GLU:OE2	1:A:471:TRP:HZ2	2.05	0.40
1:C:729:TYR:HE1	1:C:753:LYS:HB3	1.86	0.40
2:F:71:MET:C	2:F:73:ALA:H	2.25	0.40
1:C:338:LEU:HG	1:C:343:VAL:HG21	2.03	0.40
2:F:33:GLY:O	2:F:35:VAL:N	2.54	0.40
1:B:500:SER:O	1:B:503:GLU:N	2.54	0.40
1:B:550:SER:OG	1:B:553:GLN:CG	2.67	0.40
1:A:750:GLN:CG	1:A:751:TYR:N	2.82	0.40
1:B:649:ILE:O	1:B:651:LYS:N	2.54	0.40
2:E:121:VAL:C	2:E:123:GLU:N	2.74	0.40
1:C:657:ILE:HG13	1:C:759:GLN:CB	2.51	0.40
1:A:735:VAL:C	1:A:737:LYS:H	2.25	0.40
1:A:310:GLU:CG	1:A:340:LYS:NZ	2.84	0.40
1:C:369:ASP:O	1:C:374:HIS:HB2	2.22	0.40
1:A:706:ASN:C	1:A:708:ALA:N	2.75	0.40
1:B:738:SER:HB3	1:B:739:LYS:H	1.60	0.40
1:B:320:ARG:HA	1:B:598:PRO:O	2.22	0.40
2:E:130:ILE:CG2	2:E:130:ILE:O	2.70	0.40
1:B:406:ASP:O	1:B:408:LEU:N	2.54	0.40
1:C:664:ILE:HG23	2:F:14:GLU:HB2	2.04	0.40
1:B:333:LYS:O	1:B:336:THR:HG22	2.21	0.40
1:B:517:VAL:O	1:B:517:VAL:HG22	2.21	0.40
1:C:360:VAL:HG21	1:C:365:PRO:HB3	2.03	0.40
2:E:106:ARG:HG2	2:E:110:THR:HG21	2.02	0.40
1:C:655:ASN:ND2	1:C:655:ASN:N	2.69	0.40

There are no symmetry-related clashes.

## 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	475/510 (93%)	371 (78%)	83 (18%)	21 (4%)	3	24
1	B	448/510 (88%)	308 (69%)	116 (26%)	24 (5%)	2	19
1	C	477/510 (94%)	358 (75%)	98 (20%)	21 (4%)	3	24
2	D	141/148 (95%)	85 (60%)	43 (30%)	13 (9%)	1	5
2	E	141/148 (95%)	87 (62%)	37 (26%)	17 (12%)	0	2
2	F	141/148 (95%)	88 (62%)	36 (26%)	17 (12%)	0	2
All	All	1823/1974 (92%)	1297 (71%)	413 (23%)	113 (6%)	2	14

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	521	ASN
1	A	539	GLU
1	A	669	SER
2	D	81	SER
1	B	428	ASN
1	B	503	GLU
1	B	566	TYR
2	E	20	ASP
2	E	25	GLY
1	C	330	PRO
1	C	510	GLN
2	F	86	ARG
1	A	374	HIS
1	A	407	HIS
1	A	510	GLN
1	A	578	GLY
1	A	668	SER
1	A	797	ILE
2	D	17	SER
2	D	25	GLY
2	D	41	GLN
1	B	449	GLU
1	B	510	GLN
1	B	608	TRP
1	B	634	LYS
1	B	654	ILE
2	E	81	SER
2	E	82	GLU
2	E	93	ASP

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Mol	Chain	Res	Type
2	E	114	GLU
2	E	118	ASP
1	C	296	LEU
1	C	348	LEU
1	C	651	LYS
1	C	765	THR
1	C	776	LEU
1	C	796	ILE
2	F	20	ASP
2	F	25	GLY
2	F	57	ALA
2	F	144	MET
1	A	471	TRP
1	A	506	LYS
1	A	571	GLY
1	A	670	ILE
1	A	707	SER
1	A	710	HIS
1	A	780	LEU
2	D	31	GLU
2	D	54	GLU
2	D	80	ASP
1	B	373	LYS
1	B	377	GLN
1	B	384	ASN
1	B	506	LYS
1	B	526	GLN
1	B	640	LYS
1	B	746	LYS
1	B	756	ILE
1	B	757	THR
2	E	21	LYS
2	E	59	GLY
2	E	74	ARG
2	E	76	MET
2	E	106	ARG
1	C	368	GLN
1	C	428	ASN
1	C	482	GLU
1	C	520	PRO
1	C	578	GLY
2	F	8	GLN

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Mol	Chain	Res	Type
2	F	39	LEU
2	F	45	GLU
2	F	74	ARG
2	F	122	ASP
1	A	518	ASN
1	A	753	LYS
2	D	9	ILE
2	D	12	PHE
2	D	86	ARG
1	B	607	ASN
1	B	648	PRO
1	B	650	THR
2	E	65	PHE
2	E	66	PRO
2	E	121	VAL
1	C	407	HIS
1	C	569	TYR
1	C	648	PRO
2	F	67	GLU
2	F	107	HIS
2	D	27	ILE
2	D	61	GLY
1	B	507	GLN
1	B	630	ARG
2	E	8	GLN
1	C	740	GLN
2	F	50	ASP
2	F	137	ASN
1	A	598	PRO
1	B	571	GLY
1	B	629	ASN
1	C	316	LYS
1	C	537	GLY
1	C	719	LYS
2	D	65	PHE
2	F	85	ILE
1	A	732	ILE
2	E	27	ILE
1	C	350	VAL
2	F	43	PRO
2	F	108	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/455 (94%)	395 (92%)	34 (8%)	15	53
1	B	405/455 (89%)	350 (86%)	55 (14%)	5	22
1	C	431/455 (95%)	397 (92%)	34 (8%)	15	53
2	D	121/126 (96%)	112 (93%)	9 (7%)	17	56
2	E	121/126 (96%)	114 (94%)	7 (6%)	25	66
2	F	121/126 (96%)	119 (98%)	2 (2%)	68	90
All	All	1628/1743 (93%)	1487 (91%)	141 (9%)	13	45

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	A	302	LEU
1	A	332	ASN
1	A	349	ASN
1	A	434	LEU
1	A	439	ASN
1	A	440	GLN
1	A	444	PHE
1	A	445	ARG
1	A	449	GLU
1	A	455	TYR
1	A	479	LYS
1	A	482	GLU
1	A	494	LEU
1	A	531	ASN
1	A	544	SER
1	A	549	LEU
1	A	574	VAL
1	A	576	ASN
1	A	579	THR
1	A	603	ILE
1	A	604	LEU

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Mol	Chain	Res	Type
1	A	613	ARG
1	A	620	THR
1	A	622	LYS
1	A	629	ASN
1	A	639	ASN
1	A	644	GLU
1	A	656	THR
1	A	695	LYS
1	A	715	GLU
1	A	736	LEU
1	A	747	ASN
1	A	762	LEU
2	D	22	ASP
2	D	32	LEU
2	D	65	PHE
2	D	94	LYS
2	D	99	TYR
2	D	107	HIS
2	D	118	ASP
2	D	119	GLU
2	D	123	GLU
1	B	307	LEU
1	B	315	PHE
1	B	316	LYS
1	B	320	ARG
1	B	324	THR
1	B	332	ASN
1	B	336	THR
1	B	337	ASN
1	B	345	THR
1	B	360	VAL
1	B	367	ASP
1	B	385	LEU
1	B	389	LYS
1	B	400	LYS
1	B	414	LYS
1	B	416	ASN
1	B	427	ASP
1	B	428	ASN
1	B	433	TYR
1	B	436	GLU
1	B	440	GLN

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Mol	Chain	Res	Type
1	B	445	ARG
1	B	450	ASN
1	B	455	TYR
1	B	464	VAL
1	B	479	LYS
1	B	488	LEU
1	B	501	LEU
1	B	533	LEU
1	B	536	TYR
1	B	539	GLU
1	B	540	ARG
1	B	543	ASP
1	B	545	THR
1	B	549	LEU
1	B	552	TRP
1	B	556	MET
1	B	559	ARG
1	B	566	TYR
1	B	576	ASN
1	B	588	GLU
1	B	590	ASP
1	B	595	ILE
1	B	609	GLU
1	B	610	MET
1	B	628	PHE
1	B	631	SER
1	B	634	LYS
1	B	639	ASN
1	B	646	THR
1	B	709	ASN
1	B	730	ASN
1	B	739	LYS
1	B	744	GLU
1	B	784	GLU
2	E	37	ARG
2	E	58	ASP
2	E	64	ASP
2	E	76	MET
2	E	94	LYS
2	E	125	ILE
2	E	145	MET
1	C	292	ARG

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Mol	Chain	Res	Type
1	C	317	LYS
1	C	324	THR
1	C	332	ASN
1	C	341	SER
1	C	349	ASN
1	C	391	ILE
1	C	407	HIS
1	C	411	GLU
1	C	415	GLU
1	C	436	GLU
1	C	440	GLN
1	C	455	TYR
1	C	509	PRO
1	C	520	PRO
1	C	524	GLU
1	C	527	LYS
1	C	531	ASN
1	C	549	LEU
1	C	553	GLN
1	C	574	VAL
1	C	580	GLU
1	C	599	GLU
1	C	603	ILE
1	C	629	ASN
1	C	632	TYR
1	C	633	ASN
1	C	639	ASN
1	C	646	THR
1	C	648	PRO
1	C	666	ASN
1	C	737	LYS
1	C	747	ASN
1	C	780	LEU
2	F	65	PHE
2	F	78	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	A	349	ASN
1	A	377	GLN

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Mol	Chain	Res	Type
1	A	439	ASN
1	A	440	GLN
1	A	470	ASN
1	A	507	GLN
1	A	510	GLN
1	A	518	ASN
1	A	576	ASN
1	A	577	HIS
1	A	607	ASN
1	A	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	666	ASN
1	A	714	GLN
1	A	758	ASN
1	A	761	GLN
1	A	766	HIS
1	A	789	ASN
1	A	794	GLN
2	D	8	GLN
2	D	41	GLN
1	B	332	ASN
1	B	376	GLN
1	B	384	ASN
1	B	416	ASN
1	B	439	ASN
1	B	450	ASN
1	B	454	GLN
1	B	470	ASN
1	B	518	ASN
1	B	531	ASN
1	B	551	ASN
1	B	555	GLN
1	B	591	ASN
1	B	639	ASN
1	B	709	ASN
1	B	730	ASN
1	B	734	ASN
1	B	759	GLN
1	B	761	GLN
2	E	8	GLN
2	E	41	GLN

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Mol	Chain	Res	Type
2	E	135	GLN
1	C	332	ASN
1	C	337	ASN
1	C	349	ASN
1	C	376	GLN
1	C	377	GLN
1	C	440	GLN
1	C	507	GLN
1	C	510	GLN
1	C	518	ASN
1	C	531	ASN
1	C	555	GLN
1	C	618	ASN
1	C	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	655	ASN
1	C	714	GLN
1	C	759	GLN
1	C	779	GLN
1	C	781	ASN
1	C	789	ASN
1	C	794	GLN
2	F	8	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 15 are monoatomic - leaving 6 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$
5	CMP	A	289	4	19,25,25	1.70	5 (26%)	18,39,39	5.83	9 (50%)
6	POP	A	893	4	8,8,8	1.99	2 (25%)	13,13,13	1.03	1 (7%)
5	CMP	B	290	4	19,25,25	1.38	4 (21%)	18,39,39	5.29	10 (55%)
6	POP	B	894	4	8,8,8	2.17	3 (37%)	13,13,13	1.07	1 (7%)
6	POP	C	895	4	8,8,8	1.77	3 (37%)	13,13,13	1.07	1 (7%)
5	CMP	C	910	4	19,25,25	1.26	1 (5%)	18,39,39	5.01	10 (55%)

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
5	CMP	A	289	4	1/1/5/5	0/0/31/31	0/4/4/4
6	POP	A	893	4	-	0/6/6/6	0/0/0/0
5	CMP	B	290	4	1/1/5/5	0/0/31/31	0/4/4/4
6	POP	B	894	4	-	0/6/6/6	0/0/0/0
6	POP	C	895	4	-	0/6/6/6	0/0/0/0
5	CMP	C	910	4	1/1/5/5	0/0/31/31	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	289	CMP	P-O3'	-4.46	1.50	1.58
6	B	894	POP	P2-O	-4.11	1.51	1.61
6	A	893	POP	P2-O	-3.53	1.53	1.61
6	B	894	POP	P1-O	-3.15	1.53	1.61
6	C	895	POP	P1-O	-3.07	1.54	1.61
5	B	290	CMP	P-O3'	-2.99	1.53	1.58
6	A	893	POP	P1-O	-2.83	1.54	1.61
6	C	895	POP	P2-O	-2.83	1.54	1.61
5	C	910	CMP	P-O3'	-2.53	1.53	1.58
5	B	290	CMP	C8-N7	-2.44	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	289	CMP	C4-N3	-2.14	1.32	1.35
5	A	289	CMP	C8-N7	-2.08	1.30	1.34
6	C	895	POP	P1-O2	-2.08	1.46	1.55
6	B	894	POP	P1-O2	-2.03	1.47	1.55
5	B	290	CMP	C2-N3	2.22	1.36	1.32
5	A	289	CMP	C2-N3	2.34	1.36	1.32
5	B	290	CMP	O4'-C1'	2.62	1.44	1.41
5	A	289	CMP	O4'-C1'	2.96	1.45	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	290	CMP	N3-C2-N1	-11.84	119.83	128.89
5	A	289	CMP	N3-C2-N1	-11.24	120.28	128.89
5	C	910	CMP	N3-C2-N1	-10.73	120.67	128.89
5	A	289	CMP	C4'-O4'-C1'	-5.54	103.64	109.72
5	A	289	CMP	C3'-C2'-C1'	-3.75	90.97	99.98
5	A	289	CMP	O5'-P-O3'	-2.95	101.42	105.75
5	B	290	CMP	C3'-C2'-C1'	-2.82	93.20	99.98
5	B	290	CMP	C4'-O4'-C1'	-2.81	106.63	109.72
6	C	895	POP	O5-P2-O4	-2.77	100.67	110.85
6	A	893	POP	O5-P2-O4	-2.71	100.91	110.85
6	B	894	POP	O5-P2-O4	-2.64	101.17	110.85
5	A	289	CMP	C2'-C3'-C4'	-2.48	98.64	103.29
5	C	910	CMP	C3'-C2'-C1'	-2.40	94.21	99.98
5	B	290	CMP	O5'-P-O3'	-2.37	102.27	105.75
5	C	910	CMP	C4'-O4'-C1'	-2.06	107.45	109.72
5	C	910	CMP	O5'-P-O3'	-2.01	102.80	105.75
5	C	910	CMP	O3'-C3'-C4'	2.60	112.79	110.72
5	B	290	CMP	O3'-C3'-C4'	2.79	112.94	110.72
5	B	290	CMP	C2'-C1'-N9	3.40	119.48	114.29
5	C	910	CMP	C2-N1-C6	4.14	126.16	118.77
5	A	289	CMP	C2-N1-C6	4.18	126.24	118.77
5	C	910	CMP	C2'-C1'-N9	4.26	120.80	114.29
5	B	290	CMP	C2-N1-C6	4.48	126.77	118.77
5	C	910	CMP	C4-C5-N7	4.75	113.85	109.48
5	B	290	CMP	C4-C5-N7	5.54	114.58	109.48
5	A	289	CMP	C4-C5-N7	5.80	114.81	109.48
5	C	910	CMP	C1'-N9-C4	8.87	140.31	126.94
5	B	290	CMP	C1'-N9-C4	9.37	141.07	126.94
5	A	289	CMP	C1'-N9-C4	11.27	143.94	126.94
5	C	910	CMP	O4'-C1'-N9	12.88	135.06	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	B	290	CMP	O4'-C1'-N9	13.10	135.53	108.10
5	A	289	CMP	O4'-C1'-N9	15.32	140.17	108.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	910	CMP	C1'
5	A	289	CMP	C1'
5	B	290	CMP	C1'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	289	CMP	6	0
6	A	893	POP	3	0
5	B	290	CMP	5	0
6	B	894	POP	1	0
6	C	895	POP	1	0
5	C	910	CMP	3	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	481/510 (94%)	-0.07	8 (1%) 73 60	10, 43, 95, 99	0
1	B	454/510 (89%)	0.17	28 (6%) 24 13	10, 51, 95, 98	0
1	C	483/510 (94%)	-0.04	18 (3%) 45 30	10, 43, 95, 97	0
2	D	143/148 (96%)	0.84	25 (17%) 2 1	18, 95, 95, 98	0
2	E	143/148 (96%)	1.35	42 (29%) 1 0	39, 95, 96, 98	0
2	F	143/148 (96%)	0.82	25 (17%) 2 1	17, 95, 95, 97	0
All	All	1847/1974 (93%)	0.24	146 (7%) 15 9	10, 55, 95, 99	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	79	THR	9.3
2	E	59	GLY	7.9
2	E	79	THR	7.3
2	E	71	MET	7.2
1	B	740	GLN	7.1
1	B	736	LEU	6.1
1	B	779	GLN	6.1
2	E	69	LEU	5.9
1	B	778	LYS	5.9
2	F	19	PHE	5.8
2	E	78	ASP	5.3
2	F	18	LEU	5.3
1	B	780	LEU	5.2
2	E	68	PHE	5.2
2	D	59	GLY	4.9
2	E	66	PRO	4.9
2	D	19	PHE	4.9
2	D	58	ASP	4.8
2	E	17	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	E	65	PHE	4.5
1	B	422	GLY	4.4
2	E	55	VAL	4.4
2	D	29	THR	4.2
2	F	29	THR	4.2
2	E	58	ASP	4.2
2	E	15	ALA	4.2
2	D	69	LEU	4.2
2	F	28	THR	4.1
2	D	18	LEU	4.1
1	B	776	LEU	4.1
2	E	42	ASN	4.1
2	E	60	ASN	4.0
2	E	51	MET	3.8
2	D	68	PHE	3.8
1	B	783	THR	3.8
2	F	59	GLY	3.8
2	E	109	MET	3.8
2	D	60	ASN	3.7
2	F	42	ASN	3.7
2	F	23	GLY	3.6
2	D	57	ALA	3.6
2	E	19	PHE	3.6
1	B	735	VAL	3.5
2	F	45	GLU	3.5
2	F	52	ILE	3.5
2	F	17	SER	3.5
2	E	147	ALA	3.5
2	E	113	GLY	3.5
1	B	793	PHE	3.5
2	D	53	ASN	3.5
1	B	723	PHE	3.4
2	E	112	LEU	3.4
2	F	69	LEU	3.3
1	C	744	GLU	3.2
1	B	782	PHE	3.2
2	E	14	GLU	3.2
1	C	741	ILE	3.2
2	E	13	LYS	3.1
1	B	738	SER	3.1
2	D	34	THR	3.1
2	E	75	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	33	GLY	3.0
1	B	509	PRO	3.0
2	F	60	ASN	3.0
2	F	24	ASP	2.9
2	E	76	MET	2.9
2	D	76	MET	2.9
2	F	43	PRO	2.9
2	F	58	ASP	2.9
1	C	736	LEU	2.9
1	C	735	VAL	2.9
2	D	50	ASP	2.9
2	E	39	LEU	2.9
1	C	783	THR	2.9
1	B	763	LEU	2.9
1	C	782	PHE	2.9
2	E	29	THR	2.8
1	B	749	PHE	2.8
1	B	704	TYR	2.8
1	C	796	ILE	2.8
2	D	46	ALA	2.8
2	F	21	LYS	2.8
2	F	49	GLN	2.7
2	E	72	MET	2.7
1	A	798	ASP	2.7
1	A	732	ILE	2.6
2	E	41	GLN	2.6
1	B	777	TYR	2.6
2	E	16	PHE	2.6
2	F	84	GLU	2.6
2	E	23	GLY	2.6
1	B	737	LYS	2.6
1	B	741	ILE	2.6
1	C	732	ILE	2.5
2	D	78	ASP	2.5
2	E	31	GLU	2.5
2	E	102	ALA	2.5
2	D	28	THR	2.5
2	D	71	MET	2.5
2	E	24	ASP	2.5
2	E	114	GLU	2.5
1	B	513	TRP	2.5
1	C	778	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	784	GLU	2.5
2	E	12	PHE	2.5
2	F	46	ALA	2.4
2	F	51	MET	2.4
1	C	673	SER	2.4
1	A	781	ASN	2.4
1	B	508	ILE	2.4
1	B	425	GLU	2.4
1	C	739	LYS	2.4
2	D	65	PHE	2.4
2	E	70	THR	2.3
1	C	785	ASN	2.3
2	F	53	ASN	2.3
1	C	780	LEU	2.3
1	B	766	HIS	2.3
2	F	78	ASP	2.3
1	C	521	ASN	2.3
1	C	520	PRO	2.3
1	A	729	TYR	2.3
2	D	48	LEU	2.3
2	D	52	ILE	2.3
1	A	782	PHE	2.3
2	D	14	GLU	2.2
2	E	34	THR	2.2
2	F	79	THR	2.2
2	E	18	LEU	2.2
2	E	28	THR	2.2
1	C	740	GLN	2.2
2	E	49	GLN	2.2
1	B	739	LYS	2.2
1	A	736	LEU	2.2
2	E	110	THR	2.2
1	B	785	ASN	2.1
1	B	725	GLY	2.1
1	A	739	LYS	2.1
2	F	30	LYS	2.1
1	C	742	ALA	2.1
1	A	539	GLU	2.1
2	E	121	VAL	2.1
2	D	17	SER	2.1
1	B	705	TYR	2.0
2	D	73	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	34	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	YB	B	908	1/1	0.95	0.36	4.15	49,49,49,49	1
4	YB	B	905	1/1	0.98	0.35	3.86	31,31,31,31	1
4	YB	A	907	1/1	0.95	0.35	3.67	49,49,49,49	1
3	CA	F	805	1/1	0.96	0.33	3.19	21,21,21,21	0
6	POP	A	893	9/9	0.94	0.29	2.89	96,101,104,105	0
3	CA	D	801	1/1	0.98	0.35	2.20	13,13,13,13	0
6	POP	C	895	9/9	0.88	0.30	1.65	50,52,61,62	0
6	POP	B	894	9/9	0.93	0.26	1.41	51,52,54,55	0
5	CMP	C	910	22/22	0.87	0.28	1.23	15,22,44,45	0
3	CA	E	803	1/1	0.99	0.32	1.17	23,23,23,23	0
5	CMP	A	289	22/22	0.91	0.25	1.13	11,18,39,43	0
5	CMP	B	290	22/22	0.92	0.24	0.56	16,25,44,46	0
3	CA	F	804	1/1	0.99	0.11	-1.95	26,26,26,26	0
3	CA	D	800	1/1	0.97	0.15	-2.90	11,11,11,11	0
3	CA	E	802	1/1	0.96	0.04	-3.16	43,43,43,43	0
4	YB	C	909	1/1	0.93	0.42	-	72,72,72,72	1
4	YB	C	906	1/1	0.97	0.40	-	31,31,31,31	1
4	YB	A	901	1/1	0.97	0.27	-	50,50,50,50	1
4	YB	B	902	1/1	0.98	0.34	-	107,107,107,107	1
4	YB	A	904	1/1	0.95	0.37	-	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	YB	C	903	1/1	0.97	0.45	-	72,72,72,72	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.