



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:20 am GMT

PDB ID : 5C78  
Title : ATP-driven lipid-linked oligosaccharide flippase PglK in apo-inward state (1)  
Authors : Perez, C.; Locher, K.P.  
Deposited on : 2015-06-24  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

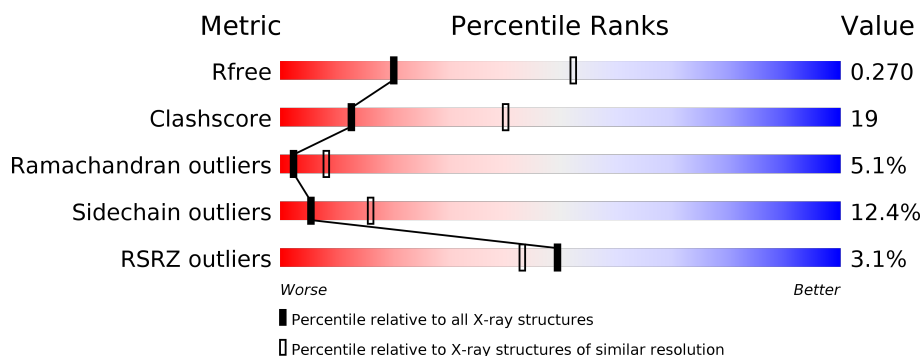
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	564	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>36%</div> <div>9%</div> </div> </div>
1	B	564	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>9%</div> </div> </div>
1	C	564	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>37%</div> <div>8%</div> </div> </div>
1	D	564	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18423 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 ATP-driven flippase PglK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	B	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	C	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	D	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	conflict	UNP O86150
A	105	LYS	TYR	conflict	UNP O86150
A	510	GLN	GLU	conflict	UNP O86150
B	2	VAL	LEU	conflict	UNP O86150
B	105	LYS	TYR	conflict	UNP O86150
B	510	GLN	GLU	conflict	UNP O86150
C	2	VAL	LEU	conflict	UNP O86150
C	105	LYS	TYR	conflict	UNP O86150
C	510	GLN	GLU	conflict	UNP O86150
D	2	VAL	LEU	conflict	UNP O86150
D	105	LYS	TYR	conflict	UNP O86150
D	510	GLN	GLU	conflict	UNP O86150

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



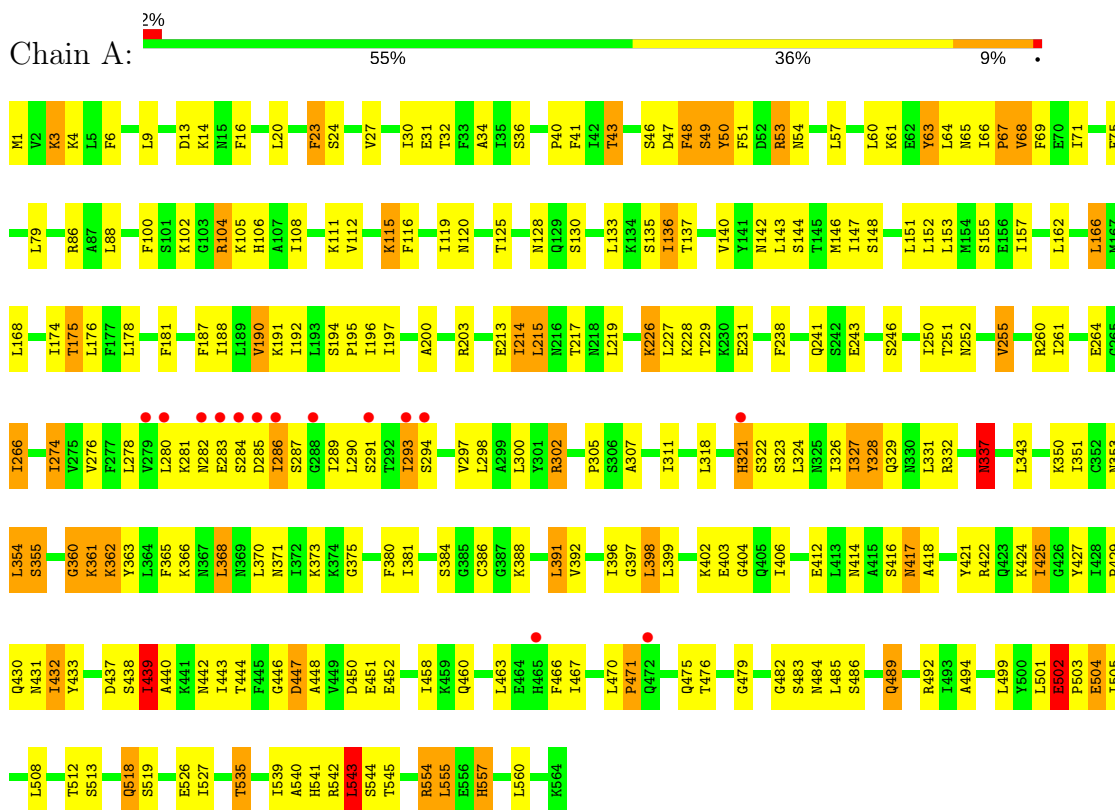
- Molecule 3 is water.



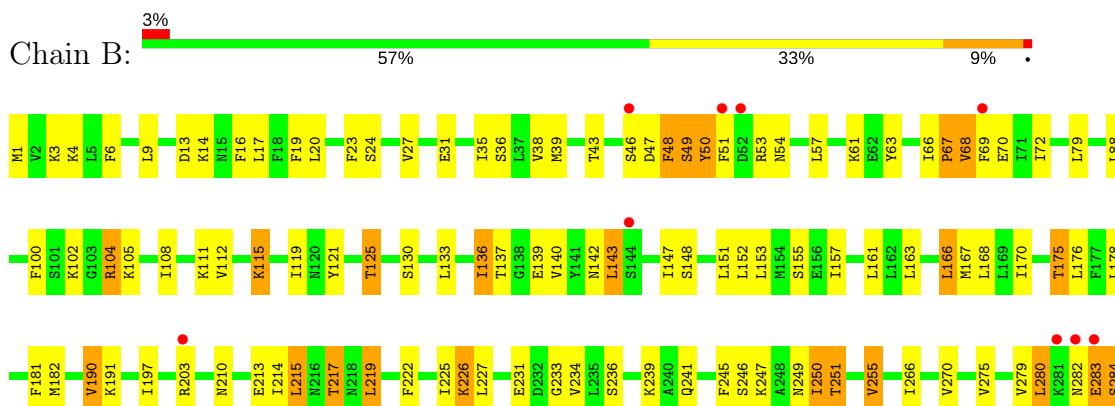
### 3 Residue-property plots

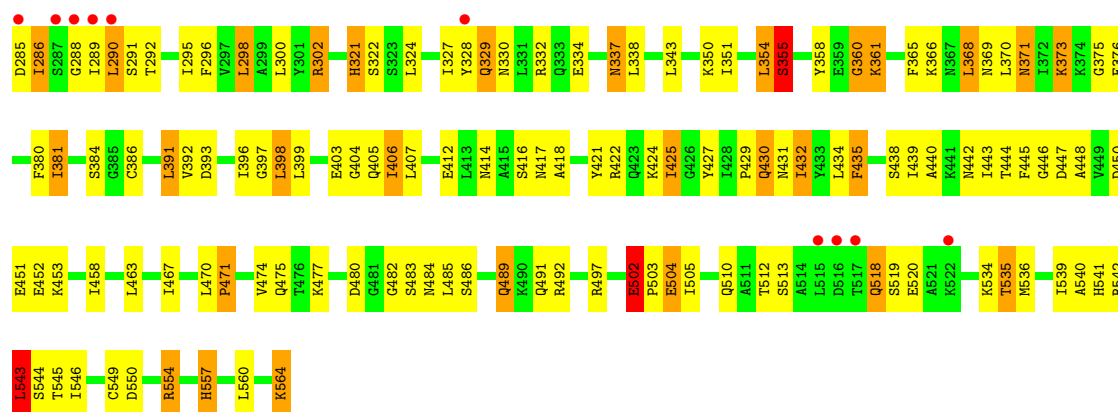
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: ATP-driven flippase PgIK

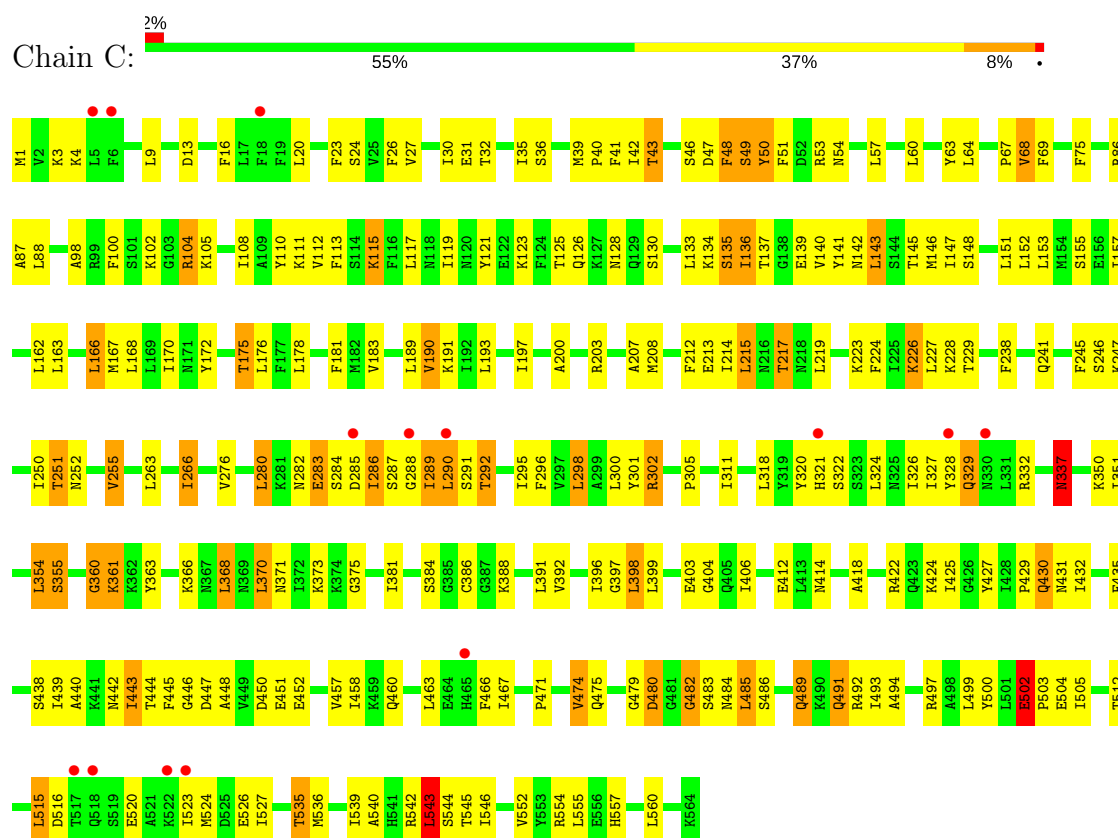


#### • Molecule 1: ATP-driven flippase PgIK

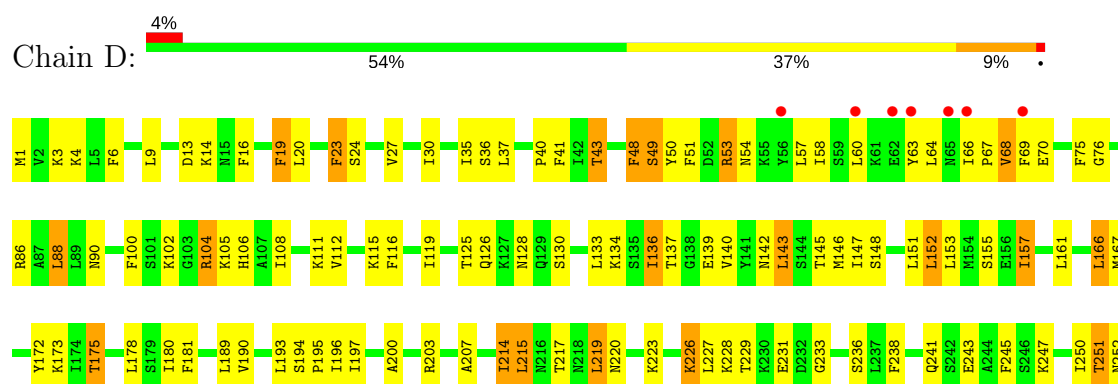


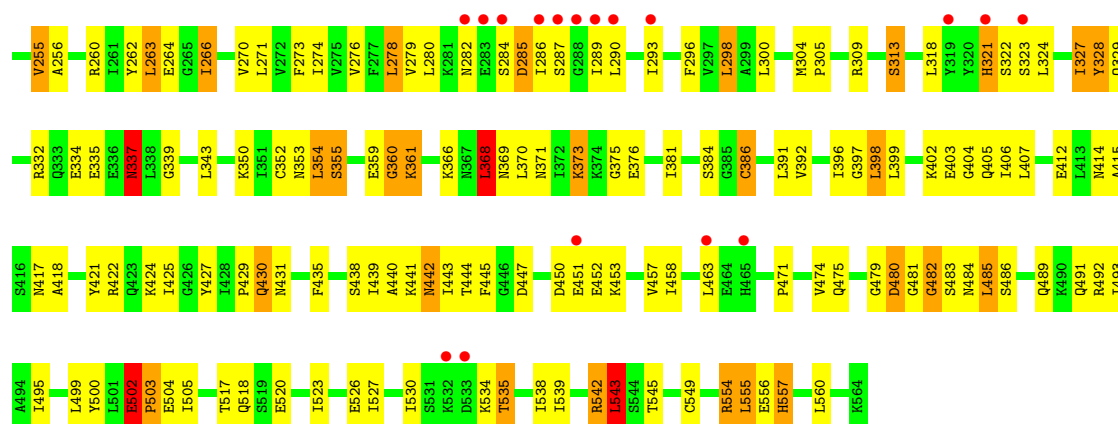


• Molecule 1: ATP-driven flippase PgIk



• Molecule 1: ATP-driven flippase PgIk





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.60Å 114.42Å 145.59Å 68.44° 73.27° 68.67°	Depositor
Resolution (Å)	27.93 – 2.90 49.48 – 2.81	Depositor EDS
% Data completeness (in resolution range)	87.2 (27.93-2.90) 80.3 (49.48-2.81)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.232 , 0.267 0.238 , 0.270	Depositor DCC
$R_{free}$ test set	5133 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	18423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE

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	0.55	2/4641 (0.0%)	0.75	1/6246 (0.0%)
1	B	0.52	0/4641	0.73	1/6246 (0.0%)
1	C	0.55	1/4641 (0.0%)	0.73	1/6246 (0.0%)
1	D	0.56	1/4641 (0.0%)	0.78	3/6246 (0.0%)
All	All	0.55	4/18564 (0.0%)	0.75	6/24984 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	TYR	CB-CG	-5.62	1.43	1.51
1	C	337	ASN	CB-CG	5.10	1.62	1.51
1	D	328	TYR	CB-CG	-5.07	1.44	1.51
1	A	328	TYR	CD1-CE1	-5.04	1.31	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	LEU	CA-CB-CG	6.18	129.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	543	LEU	N-CA-C	-5.77	95.41	111.00
1	B	543	LEU	N-CA-C	-5.70	95.62	111.00
1	D	482	GLY	N-CA-C	-5.22	100.05	113.10
1	A	543	LEU	N-CA-C	-5.20	96.97	111.00
1	C	482	GLY	N-CA-C	-5.09	100.36	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	502	GLU	Peptide
1	B	502	GLU	Peptide
1	C	502	GLU	Peptide
1	D	502	GLU	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	4557	0	4764	182	0
1	B	4557	0	4764	185	0
1	C	4557	0	4764	183	0
1	D	4557	0	4764	191	0
2	A	16	0	22	0	0
2	B	32	0	44	1	0
2	C	16	0	22	1	0
2	D	16	0	22	1	0
3	A	27	0	0	0	0
3	B	26	0	0	1	0
3	C	27	0	0	0	0
3	D	35	0	0	5	0
All	All	18423	0	19166	695	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 19.

All (695) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HG3	1:A:329:GLN:HG3	1.44	1.00
1:C:4:LYS:HG3	1:C:329:GLN:HG3	1.45	0.98
1:B:4:LYS:HG3	1:B:329:GLN:HG3	1.46	0.98
1:D:4:LYS:HG3	1:D:329:GLN:HG3	1.48	0.95
1:B:119:ILE:O	1:C:226:LYS:NZ	2.00	0.94
1:A:425:ILE:HG22	1:A:505:ILE:HB	1.48	0.94
1:D:425:ILE:HG22	1:D:505:ILE:HB	1.50	0.93
1:C:425:ILE:HG22	1:C:505:ILE:HB	1.48	0.93
1:C:355:SER:HB2	1:C:403:GLU:HB2	1.48	0.93
1:D:355:SER:HB2	1:D:403:GLU:HB2	1.52	0.92
1:B:425:ILE:HG22	1:B:505:ILE:HB	1.53	0.90
1:C:214:ILE:HD11	1:C:238:PHE:HA	1.57	0.87
1:A:486:SER:OG	1:A:489:GLN:NE2	2.09	0.86
1:A:49:SER:O	1:A:51:PHE:N	2.08	0.85
1:B:49:SER:O	1:B:51:PHE:N	2.10	0.84
1:D:49:SER:O	1:D:51:PHE:N	2.12	0.83
1:A:375:GLY:H	1:A:535:THR:HB	1.43	0.83
1:D:520:GLU:OE2	1:D:542:ARG:NH1	2.11	0.83
1:A:438:SER:O	1:A:440:ALA:N	2.13	0.82
1:A:215:LEU:HD21	1:D:136:ILE:HD11	1.63	0.81
1:A:397:GLY:HA3	1:A:422:ARG:HD2	1.63	0.80
1:B:397:GLY:HA3	1:B:422:ARG:HD2	1.64	0.80
1:C:438:SER:O	1:C:440:ALA:N	2.16	0.79
1:B:412:GLU:HG2	1:B:414:ASN:HD22	1.46	0.79
1:B:48:PHE:HE1	1:B:68:VAL:HB	1.46	0.79
1:D:375:GLY:H	1:D:535:THR:HB	1.48	0.78
1:B:51:PHE:HB3	1:B:61:LYS:HG3	1.66	0.78
1:C:450:ASP:O	1:C:452:GLU:N	2.16	0.78
1:C:49:SER:O	1:C:51:PHE:N	2.17	0.77
1:B:438:SER:O	1:B:440:ALA:N	2.18	0.76
1:A:188:ILE:HA	1:A:192:ILE:HD12	1.67	0.76
1:D:438:SER:O	1:D:440:ALA:N	2.18	0.76
1:B:227:LEU:HD22	1:C:425:ILE:HD11	1.67	0.75
1:D:1:MET:HA	1:D:4:LYS:HD3	1.69	0.75
1:A:492:ARG:NH1	1:A:526:GLU:OE1	2.20	0.74
1:B:503:PRO:HB2	1:B:504:GLU:HG2	1.69	0.73
1:C:502:GLU:HB2	1:C:503:PRO:HD3	1.69	0.73
1:C:486:SER:OG	1:C:489:GLN:OE1	2.05	0.73
1:D:412:GLU:HG2	1:D:414:ASN:HD22	1.53	0.73
1:D:430:GLN:HG2	1:D:491:GLN:HE22	1.54	0.73
1:B:360:GLY:HA3	1:B:361:LYS:HB2	1.69	0.73
1:B:286:ILE:HG21	1:C:286:ILE:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HB2	1:A:560:LEU:HD12	1.70	0.72
1:A:13:ASP:OD1	1:A:104:ARG:NH1	2.23	0.72
1:A:427:TYR:HE2	1:A:429:PRO:HB3	1.54	0.72
1:D:450:ASP:O	1:D:452:GLU:N	2.23	0.72
1:B:48:PHE:CE1	1:B:68:VAL:HB	2.24	0.72
1:D:503:PRO:HB2	1:D:504:GLU:HG2	1.70	0.72
1:A:250:ILE:HG22	1:D:102:LYS:HB2	1.73	0.71
1:C:1:MET:HA	1:C:4:LYS:HD3	1.72	0.71
1:A:291:SER:O	1:A:294:SER:OG	2.09	0.71
1:D:424:LYS:HB2	1:D:504:GLU:HG3	1.72	0.71
1:B:350:LYS:HA	1:B:371:ASN:HB3	1.73	0.70
1:C:197:ILE:HD13	1:C:255:VAL:HG13	1.72	0.70
1:A:414:ASN:OD1	1:A:416:SER:OG	2.10	0.70
1:B:450:ASP:O	1:B:452:GLU:N	2.25	0.70
1:B:424:LYS:HB2	1:B:504:GLU:HG3	1.73	0.70
1:B:375:GLY:H	1:B:535:THR:HB	1.57	0.69
1:C:111:LYS:HB3	1:C:332:ARG:HH12	1.57	0.69
1:D:430:GLN:N	3:D:701:HOH:O	2.10	0.69
1:D:502:GLU:HB2	1:D:503:PRO:HD3	1.73	0.69
1:B:250:ILE:HG22	1:C:102:LYS:HB2	1.75	0.69
1:D:335:GLU:CD	1:D:335:GLU:H	1.96	0.68
1:B:442:ASN:O	1:B:444:THR:N	2.26	0.68
1:A:36:SER:HB3	1:A:166:LEU:HD11	1.74	0.68
1:C:555:LEU:HB2	1:C:560:LEU:HD12	1.75	0.68
1:C:427:TYR:HE2	1:C:429:PRO:HB3	1.59	0.67
1:D:19:PHE:HE1	1:D:23:PHE:HD2	1.42	0.67
1:D:290:LEU:HA	1:D:293:ILE:HG22	1.75	0.67
1:D:430:GLN:HG2	1:D:491:GLN:NE2	2.09	0.67
1:C:492:ARG:NH1	1:C:526:GLU:OE1	2.27	0.67
1:C:442:ASN:O	1:C:445:PHE:N	2.19	0.67
1:D:397:GLY:HA3	1:D:422:ARG:HD2	1.76	0.66
1:C:112:VAL:HG12	1:C:136:ILE:HG22	1.77	0.66
1:C:503:PRO:HB2	1:C:504:GLU:HG2	1.76	0.66
1:D:442:ASN:O	1:D:444:THR:N	2.29	0.66
1:A:328:TYR:O	1:A:332:ARG:HG2	1.96	0.65
1:A:227:LEU:HD22	1:D:425:ILE:HD11	1.78	0.65
1:D:115:LYS:HD2	1:D:334:GLU:HB3	1.78	0.65
1:A:9:LEU:HD22	1:A:13:ASP:HB3	1.79	0.65
1:A:518:GLN:OE1	1:A:519:SER:N	2.23	0.65
1:D:178:LEU:HD13	1:D:300:LEU:HD11	1.79	0.65
1:D:492:ARG:NH1	1:D:526:GLU:OE1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:O	1:A:112:VAL:HG23	1.97	0.65
1:C:115:LYS:HG2	1:C:332:ARG:HA	1.79	0.65
1:D:146:MET:SD	1:D:321:HIS:ND1	2.67	0.65
1:B:502:GLU:HB2	1:B:503:PRO:HD3	1.79	0.64
1:C:427:TYR:CE2	1:C:429:PRO:HB3	2.32	0.64
1:D:427:TYR:HE2	1:D:429:PRO:HB3	1.60	0.64
1:B:69:PHE:HE2	1:C:282:ASN:HD22	1.45	0.64
1:C:146:MET:SD	1:C:321:HIS:ND1	2.66	0.64
1:A:20:LEU:HB3	1:A:151:LEU:HD13	1.79	0.64
1:D:197:ILE:HD13	1:D:255:VAL:HG13	1.80	0.64
1:D:427:TYR:CE2	1:D:429:PRO:HB3	2.34	0.64
1:C:375:GLY:H	1:C:535:THR:HB	1.63	0.63
1:C:190:VAL:HG13	1:C:191:LYS:HG2	1.80	0.63
1:A:354:LEU:HA	1:A:404:GLY:HA3	1.81	0.63
1:A:424:LYS:HB2	1:A:504:GLU:HG3	1.80	0.63
1:B:328:TYR:O	1:B:332:ARG:HG2	1.99	0.63
1:A:285:ASP:O	1:A:287:SER:N	2.32	0.63
1:A:503:PRO:HB2	1:A:504:GLU:HG2	1.79	0.63
1:B:215:LEU:HD13	1:C:133:LEU:HD11	1.80	0.63
1:A:412:GLU:HG2	1:A:414:ASN:HD22	1.63	0.63
1:A:243:GLU:HG3	1:D:106:HIS:CE1	2.33	0.63
1:A:112:VAL:HG22	1:A:332:ARG:HH21	1.64	0.62
1:A:102:LYS:HB2	1:D:250:ILE:HG22	1.81	0.62
1:A:140:VAL:HG22	1:A:328:TYR:OH	2.00	0.62
1:A:392:VAL:HG21	1:A:539:ILE:HG12	1.82	0.62
1:A:355:SER:HB2	1:A:403:GLU:HB2	1.81	0.62
1:B:139:GLU:O	1:B:328:TYR:OH	2.17	0.62
1:D:115:LYS:HG2	1:D:332:ARG:HA	1.81	0.62
1:D:9:LEU:HD22	1:D:13:ASP:HB3	1.81	0.62
1:A:450:ASP:O	1:A:452:GLU:N	2.32	0.62
1:B:36:SER:HB3	1:B:166:LEU:HD11	1.81	0.62
1:B:520:GLU:OE1	1:B:542:ARG:NH1	2.32	0.62
1:B:1:MET:HA	1:B:4:LYS:HD3	1.80	0.62
1:C:397:GLY:HA3	1:C:422:ARG:HD2	1.81	0.62
1:A:200:ALA:HB1	1:A:252:ASN:HA	1.82	0.61
1:A:486:SER:HG	1:A:489:GLN:HE22	1.42	0.61
1:B:16:PHE:CD2	1:B:100:PHE:HD1	2.18	0.61
1:C:354:LEU:HA	1:C:404:GLY:HA3	1.81	0.61
1:B:197:ILE:HD13	1:B:255:VAL:HG13	1.82	0.61
1:B:181:PHE:HZ	1:B:266:ILE:HG13	1.66	0.61
1:A:427:TYR:CE2	1:A:429:PRO:HB3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:SER:OG	1:C:484:ASN:N	2.33	0.61
1:A:502:GLU:HB2	1:A:503:PRO:HD3	1.83	0.61
1:C:139:GLU:O	1:C:328:TYR:OH	2.18	0.61
1:D:214:ILE:HD11	1:D:238:PHE:HA	1.83	0.61
1:D:458:ILE:HG23	1:D:463:LEU:HB2	1.82	0.61
1:A:136:ILE:HD11	1:D:215:LEU:HD11	1.82	0.60
1:D:48:PHE:HE1	1:D:68:VAL:HB	1.66	0.60
1:A:360:GLY:CA	1:A:361:LYS:HB2	2.31	0.60
1:B:483:SER:OG	1:B:484:ASN:N	2.32	0.60
1:D:153:LEU:O	1:D:157:ILE:HG23	2.00	0.60
1:A:48:PHE:HE1	1:A:68:VAL:HB	1.67	0.60
1:C:20:LEU:HB3	1:C:151:LEU:HD13	1.83	0.60
1:B:435:PHE:H	1:B:442:ASN:HD21	1.49	0.60
1:A:354:LEU:HB2	1:A:368:LEU:HB3	1.82	0.59
1:C:181:PHE:HZ	1:C:266:ILE:HG13	1.66	0.59
1:C:282:ASN:O	1:C:283:GLU:HB2	2.01	0.59
1:C:412:GLU:HG2	1:C:414:ASN:HD22	1.67	0.59
1:A:283:GLU:O	1:A:285:ASP:N	2.35	0.59
1:D:200:ALA:HB1	1:D:252:ASN:HA	1.84	0.59
1:D:492:ARG:NH1	1:D:523:ILE:HG12	2.17	0.59
1:C:438:SER:HB2	1:C:475:GLN:HA	1.84	0.59
1:A:112:VAL:HG12	1:A:136:ILE:HG22	1.85	0.59
1:B:543:LEU:O	1:B:545:THR:N	2.35	0.59
1:D:51:PHE:CE1	1:D:57:LEU:HD12	2.37	0.59
1:A:168:LEU:HA	1:A:175:THR:HG21	1.85	0.59
1:B:175:THR:HG22	1:B:296:PHE:HZ	1.67	0.59
1:C:178:LEU:HD13	1:C:300:LEU:HD11	1.85	0.59
1:D:108:ILE:O	1:D:112:VAL:HG23	2.03	0.59
1:C:424:LYS:HB2	1:C:504:GLU:HG3	1.84	0.59
1:A:281:LYS:O	1:A:283:GLU:N	2.36	0.58
1:B:368:LEU:HD11	1:B:560:LEU:HD22	1.84	0.58
1:D:518:GLN:H	1:D:518:GLN:CD	2.05	0.58
1:C:418:ALA:O	1:C:422:ARG:HD3	2.03	0.58
1:C:457:VAL:HG21	1:C:500:TYR:HA	1.84	0.58
1:B:354:LEU:HB2	1:B:368:LEU:HB3	1.86	0.58
1:B:421:TYR:O	1:B:424:LYS:HG2	2.02	0.58
1:A:31:GLU:HG3	1:A:302:ARG:HH22	1.68	0.58
1:C:350:LYS:HA	1:C:371:ASN:HB3	1.85	0.58
1:D:143:LEU:O	1:D:147:ILE:HG13	2.04	0.58
1:B:557:HIS:O	1:B:557:HIS:ND1	2.36	0.57
1:B:136:ILE:HD11	1:C:215:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:HG23	1:D:298:LEU:HB3	1.85	0.57
1:D:375:GLY:N	1:D:535:THR:HB	2.18	0.57
1:A:49:SER:OG	1:A:53:ARG:NE	2.38	0.57
1:C:142:ASN:HD22	1:C:324:LEU:HD21	1.69	0.57
1:C:392:VAL:O	1:C:396:ILE:HG12	2.04	0.57
1:C:432:ILE:HD13	1:C:494:ALA:HB2	1.85	0.57
1:B:360:GLY:CA	1:B:361:LYS:HB2	2.34	0.57
1:D:392:VAL:O	1:D:396:ILE:HG12	2.04	0.57
1:A:215:LEU:HD13	1:D:133:LEU:HD11	1.85	0.57
1:A:100:PHE:HE2	1:A:147:ILE:HG21	1.70	0.57
1:D:328:TYR:O	1:D:332:ARG:HG2	2.05	0.57
1:B:102:LYS:HB2	1:C:250:ILE:HG22	1.87	0.57
1:D:482:GLY:HA2	1:D:483:SER:HB3	1.87	0.57
1:C:51:PHE:CE1	1:C:57:LEU:HD12	2.39	0.57
1:A:142:ASN:HB2	1:A:324:LEU:HG	1.87	0.56
1:A:388:LYS:NZ	1:A:540:ALA:O	2.31	0.56
1:C:16:PHE:CD2	1:C:100:PHE:HD1	2.23	0.56
1:C:502:GLU:HB2	1:C:503:PRO:CD	2.34	0.56
1:D:418:ALA:O	1:D:422:ARG:HD3	2.05	0.56
1:A:16:PHE:CD2	1:A:100:PHE:HD1	2.23	0.56
1:A:442:ASN:H	1:A:442:ASN:ND2	2.03	0.56
1:A:197:ILE:HD13	1:A:255:VAL:HG13	1.88	0.56
1:A:479:GLY:O	1:A:483:SER:HB3	2.05	0.56
1:B:49:SER:OG	1:B:50:TYR:N	2.37	0.56
1:C:141:TYR:O	1:C:145:THR:HG22	2.05	0.56
1:D:20:LEU:HB3	1:D:151:LEU:HD13	1.86	0.56
1:A:174:ILE:HD11	1:A:278:LEU:HD22	1.86	0.56
1:A:34:ALA:HB2	1:A:86:ARG:HD3	1.85	0.56
1:C:247:LYS:O	1:C:251:THR:HG23	2.06	0.56
1:A:41:PHE:HD1	1:A:75:PHE:HD2	1.52	0.56
1:D:392:VAL:HG21	1:D:539:ILE:HG12	1.87	0.56
1:B:418:ALA:O	1:B:422:ARG:HD3	2.06	0.56
1:A:447:ASP:OD2	1:D:228:LYS:NZ	2.30	0.56
1:A:512:THR:HG22	1:A:541:HIS:CD2	2.42	0.55
1:C:392:VAL:HG21	1:C:539:ILE:HG12	1.88	0.55
1:D:105:LYS:HA	1:D:140:VAL:HG12	1.89	0.55
1:D:66:ILE:HB	1:D:70:GLU:HB2	1.87	0.55
1:C:429:PRO:O	1:C:431:ASN:N	2.40	0.55
1:C:360:GLY:CA	1:C:361:LYS:HB2	2.36	0.55
1:D:485:LEU:HD21	1:D:493:ILE:HD12	1.88	0.55
1:B:181:PHE:CZ	1:B:266:ILE:HG13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:LEU:HB2	1:D:560:LEU:HD12	1.88	0.54
1:D:429:PRO:O	1:D:431:ASN:N	2.40	0.54
1:C:351:ILE:HG13	1:C:370:LEU:HG	1.89	0.54
1:D:4:LYS:CG	1:D:329:GLN:HG3	2.32	0.54
1:D:111:LYS:HB3	1:D:332:ARG:HH12	1.73	0.54
1:D:343:LEU:HD22	1:D:417:ASN:ND2	2.22	0.54
1:A:360:GLY:HA3	1:A:361:LYS:HB2	1.88	0.54
1:A:375:GLY:N	1:A:535:THR:HB	2.20	0.54
1:A:285:ASP:HB3	1:A:289:ILE:H	1.73	0.54
1:B:284:SER:C	1:B:286:ILE:H	2.11	0.54
1:A:24:SER:HB3	1:A:155:SER:HB2	1.90	0.54
1:A:368:LEU:HD11	1:A:560:LEU:HD22	1.90	0.54
1:D:373:LYS:HB2	1:D:376:GLU:HG3	1.90	0.54
1:A:146:MET:SD	1:A:321:HIS:ND1	2.77	0.54
1:A:41:PHE:HD1	1:A:75:PHE:CD2	2.26	0.53
1:D:16:PHE:CD2	1:D:100:PHE:HD1	2.26	0.53
1:D:354:LEU:HA	1:D:404:GLY:HA3	1.89	0.53
1:B:355:SER:HB2	1:B:403:GLU:HB2	1.89	0.53
1:C:482:GLY:HA2	1:C:483:SER:OG	2.07	0.53
1:C:466:PHE:CE1	1:C:489:GLN:HG2	2.43	0.53
1:D:453:LYS:HD3	1:D:500:TYR:O	2.08	0.53
1:A:442:ASN:H	1:A:442:ASN:HD22	1.54	0.53
1:B:283:GLU:O	1:B:285:ASP:N	2.41	0.53
1:B:427:TYR:HE2	1:B:429:PRO:HB3	1.73	0.53
1:C:285:ASP:O	1:C:288:GLY:N	2.41	0.53
1:C:442:ASN:H	1:C:442:ASN:ND2	2.06	0.53
1:D:133:LEU:O	1:D:137:THR:HB	2.09	0.53
1:B:427:TYR:CE2	1:B:429:PRO:HB3	2.44	0.53
1:B:215:LEU:HD21	1:C:136:ILE:HD11	1.89	0.53
1:D:48:PHE:CE1	1:D:68:VAL:HB	2.44	0.53
1:C:112:VAL:CG1	1:C:136:ILE:HG22	2.38	0.53
1:A:429:PRO:O	1:A:431:ASN:N	2.42	0.53
1:B:360:GLY:HA3	1:B:361:LYS:CB	2.39	0.53
1:B:442:ASN:O	1:B:445:PHE:N	2.23	0.53
1:A:446:GLY:O	1:A:448:ALA:N	2.42	0.53
1:B:143:LEU:O	1:B:147:ILE:HG13	2.09	0.53
1:C:354:LEU:O	1:C:404:GLY:N	2.42	0.53
1:D:543:LEU:O	1:D:545:THR:N	2.42	0.53
1:D:323:SER:O	1:D:327:ILE:HG13	2.08	0.53
1:B:24:SER:HB3	1:B:155:SER:HB2	1.90	0.52
1:B:429:PRO:O	1:B:431:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:SER:HB3	1:C:155:SER:HB2	1.91	0.52
1:C:388:LYS:NZ	1:C:540:ALA:O	2.42	0.52
1:A:326:ILE:C	1:A:328:TYR:H	2.13	0.52
1:A:380:PHE:CE1	1:A:391:LEU:HD13	2.44	0.52
1:B:178:LEU:HD13	1:B:300:LEU:HD11	1.90	0.52
1:B:215:LEU:HD13	1:C:133:LEU:CD1	2.39	0.52
1:D:111:LYS:CB	1:D:332:ARG:HH22	2.22	0.52
1:A:48:PHE:CE1	1:A:68:VAL:HB	2.44	0.52
1:B:213:GLU:O	1:B:217:THR:HG23	2.09	0.52
1:B:438:SER:HB2	1:B:475:GLN:HA	1.90	0.52
1:B:482:GLY:HA2	1:B:483:SER:OG	2.10	0.52
1:B:520:GLU:CD	1:B:542:ARG:HH12	2.13	0.52
1:C:36:SER:HB3	1:C:166:LEU:HD11	1.92	0.52
1:A:63:TYR:O	1:A:65:ASN:N	2.43	0.52
1:D:457:VAL:HG22	1:D:499:LEU:HB3	1.91	0.52
1:D:368:LEU:HD11	1:D:560:LEU:HD22	1.92	0.52
1:A:381:ILE:HG21	1:A:554:ARG:NH1	2.25	0.52
1:C:286:ILE:O	1:C:289:ILE:HG23	2.10	0.52
1:C:355:SER:CB	1:C:403:GLU:HB2	2.31	0.52
1:B:9:LEU:HD22	1:B:13:ASP:HB3	1.92	0.52
1:D:197:ILE:HD12	1:D:256:ALA:HA	1.92	0.52
1:B:20:LEU:HB3	1:B:151:LEU:HD13	1.91	0.51
1:B:543:LEU:C	1:B:545:THR:H	2.14	0.51
1:C:48:PHE:HE1	1:C:68:VAL:HB	1.76	0.51
1:A:421:TYR:O	1:A:424:LYS:HG2	2.11	0.51
1:C:320:TYR:HA	1:C:324:LEU:HD23	1.92	0.51
1:B:290:LEU:HD23	1:C:42:ILE:HD11	1.92	0.51
1:A:40:PRO:HA	1:A:43:THR:HG22	1.91	0.51
1:C:442:ASN:H	1:C:442:ASN:HD22	1.57	0.51
1:A:543:LEU:O	1:A:545:THR:N	2.43	0.51
1:D:111:LYS:HB3	1:D:332:ARG:HH22	1.75	0.51
1:B:392:VAL:HG21	1:B:539:ILE:HG12	1.92	0.51
1:A:106:HIS:CE1	1:D:243:GLU:HG3	2.46	0.51
1:A:47:ASP:OD2	1:A:49:SER:HB3	2.11	0.51
1:B:286:ILE:HG22	1:C:287:SER:HB2	1.91	0.51
1:D:279:VAL:HA	1:D:282:ASN:OD1	2.10	0.51
1:A:442:ASN:O	1:A:444:THR:N	2.43	0.51
1:A:501:LEU:HD23	3:D:707:HOH:O	2.10	0.51
1:B:167:MET:HE3	1:B:296:PHE:CE1	2.45	0.51
1:C:360:GLY:HA3	1:C:361:LYS:HB2	1.93	0.51
1:D:40:PRO:HA	1:D:43:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:GLU:HB2	1:D:503:PRO:CD	2.40	0.51
1:C:486:SER:H	1:C:489:GLN:NE2	2.09	0.51
1:D:339:GLY:HA3	1:D:415:ALA:O	2.11	0.51
1:D:354:LEU:HB2	1:D:368:LEU:HB3	1.93	0.51
1:B:290:LEU:HD13	1:B:290:LEU:O	2.11	0.50
1:A:31:GLU:HG3	1:A:302:ARG:NH2	2.26	0.50
1:B:175:THR:HG22	1:B:296:PHE:CZ	2.44	0.50
1:A:418:ALA:O	1:A:422:ARG:HD3	2.12	0.50
1:D:360:GLY:CA	1:D:361:LYS:HB2	2.41	0.50
1:A:30:ILE:HG22	1:A:86:ARG:HG3	1.92	0.50
1:C:200:ALA:HB1	1:C:252:ASN:HA	1.94	0.50
1:C:446:GLY:O	1:C:448:ALA:N	2.44	0.50
1:B:222:PHE:HE2	1:C:121:TYR:HA	1.75	0.50
1:D:309:ARG:O	1:D:313:SER:HB3	2.12	0.50
1:B:121:TYR:O	1:B:125:THR:HB	2.10	0.50
1:C:153:LEU:O	1:C:157:ILE:HG23	2.11	0.50
1:A:181:PHE:HZ	1:A:266:ILE:HD12	1.76	0.50
1:B:292:THR:O	1:B:296:PHE:HD2	1.95	0.50
1:B:111:LYS:HB3	1:B:332:ARG:HH22	1.77	0.50
1:A:362:LYS:O	1:A:362:LYS:HD2	2.11	0.50
1:C:24:SER:O	1:C:27:VAL:HG22	2.12	0.50
1:A:51:PHE:CE1	1:A:57:LEU:HD12	2.47	0.50
1:C:328:TYR:O	1:C:332:ARG:HG2	2.12	0.50
1:A:214:ILE:HD11	1:A:238:PHE:HA	1.95	0.49
1:C:32:THR:HG21	1:C:162:LEU:CB	2.42	0.49
1:C:35:ILE:HG23	1:C:298:LEU:HB3	1.94	0.49
1:D:442:ASN:H	1:D:442:ASN:HD22	1.60	0.49
1:B:354:LEU:HA	1:B:404:GLY:HA3	1.92	0.49
1:B:540:ALA:HB2	1:B:546:ILE:HG21	1.93	0.49
1:C:458:ILE:HG23	1:C:463:LEU:HB2	1.94	0.49
1:D:479:GLY:O	1:D:480:ASP:HB2	2.12	0.49
1:B:112:VAL:CG1	1:B:136:ILE:HG22	2.43	0.49
1:B:112:VAL:HG12	1:B:136:ILE:HG22	1.94	0.49
1:A:142:ASN:CB	1:A:324:LEU:HG	2.42	0.49
1:B:463:LEU:O	1:B:467:ILE:HG12	2.12	0.49
1:B:35:ILE:HG23	1:B:298:LEU:HB3	1.94	0.49
1:B:542:ARG:O	1:B:543:LEU:HB2	2.12	0.49
1:D:175:THR:HG22	1:D:296:PHE:CZ	2.47	0.49
1:C:207:ALA:HB1	1:C:245:PHE:HA	1.94	0.49
1:B:486:SER:H	1:B:489:GLN:NE2	2.11	0.49
1:C:479:GLY:O	1:C:480:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:GLU:CD	1:C:542:ARG:HH12	2.17	0.49
1:D:304:MET:HB2	1:D:305:PRO:HD3	1.93	0.49
1:B:512:THR:HG22	1:B:541:HIS:CD2	2.48	0.49
1:B:6:PHE:CD1	1:B:14:LYS:HG2	2.48	0.48
1:B:112:VAL:HG22	1:B:332:ARG:HH21	1.78	0.48
1:B:414:ASN:OD1	1:B:416:SER:OG	2.25	0.48
1:D:140:VAL:N	1:D:328:TYR:OH	2.46	0.48
1:B:425:ILE:HD11	1:C:227:LEU:HD22	1.95	0.48
1:C:520:GLU:O	1:C:524:MET:HG2	2.13	0.48
1:D:290:LEU:HA	1:D:293:ILE:CG2	2.43	0.48
1:A:396:ILE:HB	1:A:425:ILE:HD12	1.95	0.48
1:A:466:PHE:CE1	1:A:489:GLN:HG2	2.48	0.48
1:B:497:ARG:HD3	1:C:224:PHE:CZ	2.49	0.48
3:B:717:HOH:O	1:C:87:ALA:HA	2.14	0.48
1:D:142:ASN:HD22	1:D:324:LEU:HD21	1.78	0.48
1:A:392:VAL:HG11	1:A:539:ILE:HD11	1.96	0.48
1:B:380:PHE:CE1	1:B:391:LEU:HD13	2.49	0.48
1:A:427:TYR:CZ	1:D:223:LYS:HE3	2.49	0.47
1:A:463:LEU:O	1:A:467:ILE:HG12	2.14	0.47
1:C:119:ILE:HD11	1:C:123:LYS:HD3	1.95	0.47
1:C:128:ASN:N	1:C:128:ASN:OD1	2.36	0.47
1:D:233:GLY:O	1:D:236:SER:HB3	2.14	0.47
1:D:442:ASN:H	1:D:442:ASN:ND2	2.12	0.47
1:B:337:ASN:O	1:B:338:LEU:HG	2.14	0.47
1:D:134:LYS:O	1:D:139:GLU:HG2	2.14	0.47
1:A:133:LEU:HD12	1:D:215:LEU:HD13	1.96	0.47
1:A:433:TYR:CD2	1:D:220:ASN:HB3	2.49	0.47
1:B:108:ILE:O	1:B:112:VAL:HG23	2.15	0.47
1:B:373:LYS:HB2	1:B:376:GLU:HG3	1.96	0.47
1:D:350:LYS:HA	1:D:371:ASN:HB3	1.96	0.47
1:D:412:GLU:HG2	1:D:414:ASN:ND2	2.25	0.47
1:A:266:ILE:HA	1:A:266:ILE:HD13	1.66	0.47
1:B:285:ASP:CG	1:B:288:GLY:HA3	2.35	0.47
1:B:381:ILE:HD13	1:B:381:ILE:HA	1.67	0.47
1:C:167:MET:HE3	1:C:296:PHE:CE1	2.49	0.47
1:C:133:LEU:O	1:C:137:THR:HB	2.15	0.47
1:C:190:VAL:CG1	1:C:191:LYS:HG2	2.42	0.47
1:C:41:PHE:HD1	1:C:75:PHE:HD2	1.62	0.47
1:D:207:ALA:HB1	1:D:245:PHE:HA	1.96	0.47
1:D:36:SER:HB3	1:D:166:LEU:HD11	1.95	0.47
1:D:181:PHE:HZ	1:D:266:ILE:HG13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ILE:HB	1:D:425:ILE:CD1	2.44	0.47
1:A:432:ILE:HG13	1:A:433:TYR:N	2.28	0.47
1:B:227:LEU:HD23	1:C:398:LEU:HD21	1.96	0.47
1:B:266:ILE:HD12	1:B:266:ILE:HA	1.77	0.47
1:B:343:LEU:HD22	1:B:417:ASN:ND2	2.29	0.47
1:D:228:LYS:O	1:D:229:THR:HB	2.15	0.47
1:A:128:ASN:OD1	1:A:128:ASN:N	2.45	0.47
1:A:3:LYS:H	1:A:3:LYS:HD3	1.80	0.47
1:B:119:ILE:HD13	1:B:119:ILE:HG21	1.69	0.47
1:B:458:ILE:HG23	1:B:463:LEU:HB2	1.97	0.47
1:B:477:LYS:O	1:B:484:ASN:ND2	2.47	0.47
1:C:543:LEU:C	1:C:545:THR:H	2.18	0.47
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.65	0.46
1:B:412:GLU:HG2	1:B:414:ASN:ND2	2.24	0.46
1:D:273:PHE:HA	1:D:276:VAL:HG12	1.97	0.46
1:D:278:LEU:HA	1:D:278:LEU:HD22	1.58	0.46
1:D:441:LYS:HA	1:D:442:ASN:O	2.15	0.46
1:D:450:ASP:HB3	1:D:453:LYS:HB3	1.98	0.46
1:A:116:PHE:O	1:A:119:ILE:HG12	2.16	0.46
1:A:501:LEU:O	1:A:503:PRO:HD3	2.14	0.46
1:D:438:SER:HB2	1:D:475:GLN:HA	1.97	0.46
1:B:133:LEU:O	1:B:137:THR:HB	2.15	0.46
1:C:492:ARG:NH1	1:C:523:ILE:HG12	2.30	0.46
1:C:443:ILE:HA	1:C:497:ARG:HB2	1.98	0.46
1:D:13:ASP:OD1	1:D:104:ARG:NH1	2.48	0.46
1:D:324:LEU:HA	1:D:324:LEU:HD13	1.67	0.46
1:A:438:SER:HB2	1:A:475:GLN:HA	1.96	0.46
1:B:104:ARG:HD3	1:B:104:ARG:HA	1.65	0.46
1:B:247:LYS:O	1:B:251:THR:HG23	2.16	0.46
1:B:368:LEU:HD12	1:B:369:ASN:H	1.79	0.46
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.62	0.46
1:D:49:SER:OG	1:D:53:ARG:NH2	2.48	0.46
1:A:293:ILE:O	1:A:297:VAL:HG23	2.15	0.46
1:D:457:VAL:HG21	1:D:500:TYR:HA	1.98	0.46
1:D:503:PRO:HA	1:D:534:LYS:HE3	1.98	0.46
1:C:170:ILE:HD12	1:C:295:ILE:HG21	1.98	0.46
1:C:292:THR:O	1:C:296:PHE:HD2	1.99	0.46
1:D:167:MET:C	1:D:175:THR:HG21	2.35	0.46
1:A:112:VAL:CG1	1:A:136:ILE:HG22	2.44	0.46
1:C:146:MET:SD	1:C:321:HIS:HA	2.55	0.46
1:D:6:PHE:HD1	1:D:14:LYS:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:SER:HB3	1:D:155:SER:HB2	1.98	0.46
1:B:13:ASP:CG	1:B:104:ARG:HD2	2.36	0.46
1:B:210:ASN:O	1:B:214:ILE:HG22	2.15	0.46
1:B:392:VAL:O	1:B:396:ILE:HG12	2.15	0.46
1:A:153:LEU:O	1:A:157:ILE:HG23	2.16	0.46
1:A:432:ILE:HD13	1:A:494:ALA:HB2	1.98	0.46
1:B:225:ILE:HD13	1:B:234:VAL:HG21	1.98	0.46
1:D:66:ILE:HG22	1:D:70:GLU:OE1	2.16	0.46
1:B:133:LEU:HA	1:B:133:LEU:HD12	1.83	0.45
1:B:424:LYS:HE3	1:B:504:GLU:OE2	2.17	0.45
1:C:134:LYS:O	1:C:139:GLU:HG2	2.16	0.45
1:C:485:LEU:HD21	1:C:493:ILE:HD12	1.98	0.45
1:D:128:ASN:OD1	1:D:128:ASN:N	2.37	0.45
1:C:515:LEU:HA	1:C:516:ASP:HA	1.75	0.45
1:D:196:ILE:HG22	1:D:255:VAL:HG21	1.98	0.45
1:A:398:LEU:HD21	1:D:227:LEU:HD23	1.97	0.45
1:B:31:GLU:HG3	1:B:302:ARG:HH22	1.81	0.45
1:B:358:TYR:O	1:B:360:GLY:N	2.50	0.45
1:C:289:ILE:HD13	1:C:290:LEU:N	2.31	0.45
1:C:398:LEU:H	1:C:398:LEU:HG	1.21	0.45
1:A:286:ILE:HG22	1:D:287:SER:HB2	1.99	0.45
1:D:557:HIS:ND1	1:D:557:HIS:O	2.48	0.45
1:A:119:ILE:O	1:D:226:LYS:NZ	2.49	0.45
1:A:196:ILE:HG22	1:A:255:VAL:HG21	1.98	0.45
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.74	0.45
1:A:437:ASP:CG	1:A:438:SER:H	2.20	0.45
1:A:542:ARG:O	1:A:543:LEU:HB2	2.17	0.45
1:B:233:GLY:O	1:B:236:SER:HB3	2.16	0.45
1:A:67:PRO:HB2	1:A:68:VAL:H	1.63	0.45
1:B:286:ILE:HA	1:C:46:SER:HB2	1.99	0.45
1:A:213:GLU:HG2	3:D:715:HOH:O	2.17	0.45
1:A:307:ALA:O	1:A:311:ILE:HG12	2.17	0.45
1:B:226:LYS:NZ	1:C:119:ILE:O	2.47	0.45
1:C:396:ILE:HB	1:C:425:ILE:CD1	2.47	0.45
1:D:126:GLN:HB3	3:D:724:HOH:O	2.17	0.45
1:D:152:LEU:HD11	1:D:309:ARG:HD3	1.98	0.45
1:D:262:TYR:CD1	1:D:263:LEU:HD13	2.52	0.45
1:D:37:LEU:HD23	1:D:37:LEU:HA	1.80	0.45
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.83	0.45
1:A:24:SER:O	1:A:27:VAL:HG22	2.17	0.45
1:A:302:ARG:O	1:A:305:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HD21	1:A:492:ARG:HB2	1.99	0.45
1:B:376:GLU:O	1:B:550:ASP:HB2	2.17	0.45
1:D:542:ARG:HB2	1:D:543:LEU:O	2.16	0.44
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.85	0.44
1:A:323:SER:O	1:A:327:ILE:HG13	2.17	0.44
1:A:46:SER:HA	1:A:47:ASP:HA	1.71	0.44
1:B:170:ILE:HD12	1:B:295:ILE:HG21	1.98	0.44
1:B:39:MET:SD	1:B:291:SER:HB3	2.58	0.44
1:B:510:GLN:OE1	1:B:541:HIS:N	2.36	0.44
1:C:41:PHE:HB2	1:C:75:PHE:HE2	1.82	0.44
1:D:266:ILE:HD12	1:D:266:ILE:HA	1.64	0.44
1:D:505:ILE:HA	1:D:535:THR:O	2.17	0.44
1:A:260:ARG:HG3	1:A:261:ILE:N	2.32	0.44
1:B:137:THR:HG21	1:C:212:PHE:CZ	2.52	0.44
1:B:72:ILE:HD13	1:B:72:ILE:HA	1.85	0.44
1:C:163:LEU:HA	1:C:163:LEU:HD23	1.84	0.44
1:C:246:SER:O	1:C:250:ILE:HG23	2.17	0.44
1:A:32:THR:HG21	1:A:162:LEU:CB	2.47	0.44
1:B:38:VAL:HG21	1:B:298:LEU:HD21	1.99	0.44
1:D:116:PHE:O	1:D:119:ILE:HG12	2.16	0.44
1:D:386:CYS:SG	1:D:556:GLU:HA	2.58	0.44
1:B:108:ILE:HB	1:B:140:VAL:HG13	2.00	0.44
1:B:24:SER:O	1:B:27:VAL:HG22	2.18	0.44
1:B:289:ILE:HG13	1:B:290:LEU:N	2.33	0.44
1:B:405:GLN:O	1:B:406:ILE:HB	2.18	0.44
1:B:453:LYS:HE2	1:B:502:GLU:OE1	2.17	0.44
1:C:167:MET:HE3	1:C:296:PHE:HE1	1.83	0.44
1:A:215:LEU:HD11	1:D:136:ILE:HD11	2.00	0.44
1:A:427:TYR:OH	1:D:223:LYS:HE3	2.18	0.44
1:D:318:LEU:HA	1:D:318:LEU:HD23	1.71	0.44
1:A:190:VAL:CG1	1:A:191:LYS:HG2	2.47	0.44
1:A:424:LYS:HE3	1:A:504:GLU:OE2	2.18	0.44
1:B:153:LEU:O	1:B:157:ILE:HG23	2.17	0.44
1:B:245:PHE:O	1:B:249:ASN:HB2	2.17	0.44
1:B:432:ILE:HD11	1:B:434:LEU:HG	1.99	0.44
1:D:108:ILE:HB	1:D:140:VAL:HG13	2.00	0.44
1:D:425:ILE:HG21	1:D:425:ILE:HD13	1.78	0.44
1:A:112:VAL:CG2	1:A:332:ARG:HH21	2.28	0.44
1:B:46:SER:HA	1:B:47:ASP:HA	1.71	0.44
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.74	0.44
1:B:536:MET:HE3	1:B:536:MET:HB2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LEU:HD11	1:C:560:LEU:HD13	1.99	0.44
1:D:139:GLU:OE2	1:D:324:LEU:HD11	2.17	0.44
1:A:482:GLY:HA2	1:A:484:ASN:N	2.33	0.43
1:B:430:GLN:HG2	1:B:491:GLN:OE1	2.18	0.43
1:B:549:CYS:O	1:B:564:LYS:NZ	2.38	0.43
1:C:381:ILE:O	1:C:554:ARG:HA	2.18	0.43
1:D:442:ASN:O	1:D:445:PHE:N	2.31	0.43
1:A:246:SER:O	1:A:250:ILE:HG23	2.18	0.43
1:D:492:ARG:HH12	1:D:523:ILE:HG12	1.83	0.43
1:D:543:LEU:C	1:D:545:THR:H	2.20	0.43
1:A:350:LYS:HA	1:A:371:ASN:HB3	2.00	0.43
2:B:602:1PE:H161	2:B:602:1PE:H151	1.55	0.43
1:C:9:LEU:HD22	1:C:13:ASP:HB3	2.00	0.43
1:C:543:LEU:O	1:C:544:SER:OG	2.34	0.43
1:D:193:LEU:HD23	1:D:193:LEU:HA	1.67	0.43
1:D:421:TYR:O	1:D:424:LYS:HG2	2.18	0.43
1:D:30:ILE:HG22	1:D:86:ARG:HG3	1.99	0.43
1:C:113:PHE:CZ	1:C:117:LEU:HD11	2.53	0.43
1:D:359:GLU:HG3	2:D:601:1PE:H121	2.00	0.43
1:D:41:PHE:HD1	1:D:75:PHE:CD2	2.36	0.43
1:A:187:PHE:CE1	1:A:192:ILE:HD11	2.54	0.43
1:B:142:ASN:HB2	1:B:324:LEU:HG	2.00	0.43
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.64	0.43
1:B:167:MET:HE3	1:B:296:PHE:HE1	1.83	0.43
1:C:442:ASN:O	1:C:444:THR:N	2.51	0.43
1:B:405:GLN:CD	1:B:407:LEU:HD21	2.38	0.43
1:B:67:PRO:HB2	1:B:68:VAL:H	1.64	0.43
1:C:13:ASP:OD1	1:C:104:ARG:NH1	2.51	0.43
1:C:324:LEU:HA	1:C:324:LEU:HD13	1.71	0.43
1:C:142:ASN:CB	1:C:324:LEU:HG	2.48	0.43
1:A:178:LEU:HD13	1:A:300:LEU:HD11	2.01	0.43
1:C:381:ILE:HD11	1:C:546:ILE:HD13	2.01	0.43
1:D:172:TYR:CE1	1:D:173:LYS:HG3	2.53	0.43
1:D:417:ASN:N	1:D:417:ASN:OD1	2.45	0.43
1:B:381:ILE:HG21	1:B:554:ARG:NH1	2.33	0.43
1:B:66:ILE:HB	1:B:70:GLU:HB2	2.01	0.43
1:C:32:THR:HG22	1:C:163:LEU:HG	2.01	0.43
1:A:188:ILE:O	1:A:192:ILE:HB	2.18	0.43
1:A:68:VAL:HG12	1:A:71:ILE:HG21	2.00	0.43
1:B:290:LEU:HA	1:B:290:LEU:HD22	1.79	0.43
1:B:502:GLU:HB2	1:B:503:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LYS:O	1:C:229:THR:HB	2.19	0.43
1:C:49:SER:OG	1:C:50:TYR:N	2.51	0.43
1:C:48:PHE:CE1	1:C:68:VAL:HB	2.54	0.43
1:D:352:CYS:HA	1:D:369:ASN:ND2	2.34	0.43
1:D:355:SER:CB	1:D:403:GLU:HB2	2.38	0.43
1:D:483:SER:HG	1:D:484:ASN:H	1.66	0.43
1:C:355:SER:HB3	1:C:363:TYR:CD1	2.54	0.43
1:D:271:LEU:HD21	1:D:293:ILE:CD1	2.49	0.43
1:A:360:GLY:HA3	1:A:361:LYS:CB	2.49	0.42
1:A:439:ILE:HG22	1:A:476:THR:O	2.18	0.42
1:C:123:LYS:O	1:C:126:GLN:HG2	2.18	0.42
1:C:142:ASN:HB2	1:C:324:LEU:HG	2.01	0.42
1:C:208:MET:HB2	1:C:245:PHE:CE2	2.54	0.42
1:C:318:LEU:HA	1:C:318:LEU:HD23	1.83	0.42
1:C:397:GLY:O	2:C:601:1PE:H262	2.18	0.42
1:A:458:ILE:HG23	1:A:463:LEU:HB2	2.01	0.42
1:B:115:LYS:HE3	1:B:334:GLU:O	2.19	0.42
1:C:133:LEU:HD12	1:C:133:LEU:HA	1.80	0.42
1:C:168:LEU:HA	1:C:175:THR:HG21	2.01	0.42
1:A:120:ASN:HB3	1:A:337:ASN:ND2	2.34	0.42
1:A:194:SER:N	1:A:195:PRO:HD2	2.35	0.42
1:A:260:ARG:O	1:A:264:GLU:HG3	2.19	0.42
1:C:175:THR:HG22	1:C:296:PHE:HZ	1.83	0.42
1:C:214:ILE:HG13	1:C:215:LEU:N	2.34	0.42
1:C:460:GLN:HB3	1:C:499:LEU:HD23	2.00	0.42
1:D:274:ILE:O	1:D:278:LEU:HB2	2.20	0.42
1:B:105:LYS:HA	1:B:140:VAL:HG12	2.01	0.42
1:B:368:LEU:HD12	1:B:369:ASN:N	2.34	0.42
1:D:354:LEU:CB	1:D:368:LEU:HB3	2.50	0.42
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.71	0.42
1:B:225:ILE:HG12	1:C:445:PHE:HE2	1.85	0.42
1:B:354:LEU:HA	1:B:354:LEU:HD23	1.72	0.42
1:B:417:ASN:N	1:B:417:ASN:OD1	2.51	0.42
1:D:133:LEU:HA	1:D:133:LEU:HD12	1.76	0.42
1:A:140:VAL:HA	1:A:328:TYR:OH	2.18	0.42
1:A:343:LEU:HD22	1:A:417:ASN:ND2	2.34	0.42
1:A:51:PHE:HB3	1:A:61:LYS:HG3	2.01	0.42
1:B:190:VAL:CG1	1:B:191:LYS:HG2	2.49	0.42
1:B:393:ASP:O	1:B:398:LEU:O	2.38	0.42
1:A:217:THR:HG21	1:D:435:PHE:HB3	2.00	0.42
1:D:440:ALA:O	1:D:444:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HA	1:A:274:ILE:HD13	1.70	0.42
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.75	0.42
1:A:470:LEU:HA	1:A:471:PRO:HD3	1.94	0.42
1:B:503:PRO:HA	1:B:534:LYS:HE3	2.01	0.42
1:B:226:LYS:HE3	1:C:337:ASN:OD1	2.19	0.42
1:C:360:GLY:HA3	1:C:361:LYS:CB	2.50	0.42
1:D:178:LEU:HA	1:D:178:LEU:HD23	1.82	0.42
1:D:260:ARG:O	1:D:264:GLU:HG3	2.20	0.42
1:A:508:LEU:HD22	1:A:527:ILE:HD13	2.00	0.42
1:B:161:LEU:HA	1:B:161:LEU:HD23	1.89	0.42
1:B:282:ASN:O	1:B:283:GLU:HB2	2.20	0.42
1:B:564:LYS:HE2	1:B:564:LYS:HB3	1.77	0.42
1:C:213:GLU:O	1:C:217:THR:HG23	2.20	0.42
1:D:405:GLN:NE2	1:D:407:LEU:HD21	2.35	0.42
1:A:115:LYS:HG3	1:A:332:ARG:HA	2.01	0.42
1:A:354:LEU:O	1:A:404:GLY:N	2.53	0.42
1:A:438:SER:O	1:A:438:SER:OG	2.35	0.42
1:B:100:PHE:HE2	1:B:147:ILE:HG21	1.85	0.42
1:C:108:ILE:O	1:C:112:VAL:HG23	2.19	0.42
1:C:105:LYS:HA	1:C:140:VAL:HG12	2.00	0.42
1:C:189:LEU:HD23	1:C:193:LEU:HD12	2.01	0.42
1:C:276:VAL:O	1:C:280:LEU:HB2	2.19	0.42
1:D:247:LYS:O	1:D:251:THR:HG23	2.19	0.42
1:A:1:MET:HA	1:A:4:LYS:HD3	2.02	0.42
1:B:142:ASN:CB	1:B:324:LEU:HG	2.50	0.42
1:B:39:MET:HB2	1:B:295:ILE:HD11	2.02	0.42
1:C:168:LEU:HD23	1:C:168:LEU:HA	1.85	0.42
1:C:311:ILE:HG23	1:C:311:ILE:HD12	1.82	0.42
1:C:326:ILE:O	1:C:328:TYR:N	2.53	0.42
1:D:298:LEU:HD12	1:D:298:LEU:HA	1.80	0.42
1:C:41:PHE:HD1	1:C:75:PHE:CD2	2.37	0.41
1:A:228:LYS:O	1:A:229:THR:HB	2.19	0.41
1:B:215:LEU:HD22	1:B:219:LEU:HD22	2.01	0.41
1:B:227:LEU:CD2	1:C:398:LEU:HD21	2.50	0.41
1:B:324:LEU:HA	1:B:324:LEU:HD13	1.75	0.41
1:C:425:ILE:HD13	1:C:425:ILE:HG21	1.80	0.41
1:D:167:MET:HE3	1:D:296:PHE:HE1	1.84	0.41
1:D:355:SER:O	1:D:402:LYS:HB2	2.19	0.41
1:A:226:LYS:HE3	1:D:337:ASN:OD1	2.20	0.41
1:A:111:LYS:HB3	1:A:332:ARG:HH12	1.84	0.41
1:A:360:GLY:N	1:A:361:LYS:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:HB2	1:A:503:PRO:CD	2.49	0.41
1:B:470:LEU:HA	1:B:471:PRO:HD3	1.87	0.41
1:C:135:SER:HA	1:C:139:GLU:HG3	2.02	0.41
1:B:133:LEU:HD11	1:C:215:LEU:HD13	2.03	0.41
1:C:26:PHE:O	1:C:30:ILE:HG12	2.20	0.41
1:C:40:PRO:HA	1:C:43:THR:HG22	2.01	0.41
1:C:555:LEU:HB2	1:C:560:LEU:CD1	2.47	0.41
1:A:176:LEU:HD22	1:A:176:LEU:HA	1.84	0.41
1:A:190:VAL:HG13	1:A:191:LYS:HG2	2.01	0.41
1:A:365:PHE:CG	1:A:368:LEU:HD23	2.55	0.41
1:C:302:ARG:O	1:C:305:PRO:HD2	2.21	0.41
1:D:271:LEU:HD21	1:D:293:ILE:HD11	2.01	0.41
1:D:24:SER:O	1:D:27:VAL:HG22	2.21	0.41
1:D:398:LEU:H	1:D:398:LEU:HG	1.33	0.41
1:A:105:LYS:HA	1:A:140:VAL:HG12	2.02	0.41
1:A:214:ILE:HD11	1:A:238:PHE:CA	2.50	0.41
1:B:275:VAL:O	1:B:279:VAL:HG22	2.20	0.41
1:B:351:ILE:HG23	1:B:354:LEU:HG	2.03	0.41
1:A:49:SER:OG	1:A:50:TYR:N	2.52	0.41
1:B:168:LEU:HA	1:B:175:THR:HG21	2.03	0.41
1:D:194:SER:N	1:D:195:PRO:HD2	2.35	0.41
1:A:381:ILE:HD13	1:A:381:ILE:HA	1.85	0.41
1:B:446:GLY:O	1:B:448:ALA:N	2.54	0.41
1:C:98:ALA:O	1:C:102:LYS:HG2	2.21	0.41
1:D:19:PHE:C	1:D:19:PHE:CD1	2.93	0.41
1:D:354:LEU:O	1:D:404:GLY:N	2.53	0.41
1:A:363:TYR:OH	1:A:402:LYS:HD2	2.20	0.41
1:A:227:LEU:CD2	1:D:398:LEU:HD21	2.50	0.41
1:C:32:THR:HG21	1:C:162:LEU:HB2	2.02	0.41
1:A:6:PHE:CD1	1:A:14:LYS:HG2	2.56	0.41
1:A:276:VAL:HG21	1:D:76:GLY:HA3	2.03	0.41
1:B:222:PHE:CE2	1:B:226:LYS:HG3	2.56	0.41
1:B:463:LEU:HD21	1:B:492:ARG:HB2	2.03	0.41
1:C:4:LYS:CG	1:C:329:GLN:HG3	2.33	0.41
1:D:219:LEU:HA	1:D:219:LEU:HD12	1.82	0.41
1:D:480:ASP:OD2	1:D:481:GLY:N	2.50	0.41
1:A:557:HIS:O	1:A:557:HIS:ND1	2.52	0.41
1:B:321:HIS:O	1:B:324:LEU:N	2.54	0.41
1:B:518:GLN:OE1	1:B:519:SER:N	2.54	0.41
1:C:546:ILE:HD12	1:C:552:VAL:HG21	2.02	0.41
1:D:189:LEU:HD23	1:D:189:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ASP:O	1:D:289:ILE:HG12	2.20	0.41
1:D:538:ILE:HD12	1:D:549:CYS:SG	2.60	0.41
1:A:460:GLN:HB3	1:A:499:LEU:HD23	2.03	0.40
1:C:430:GLN:HG2	1:C:491:GLN:OE1	2.21	0.40
1:C:467:ILE:HG21	1:C:474:VAL:HG22	2.04	0.40
1:C:46:SER:HA	1:C:47:ASP:HA	1.70	0.40
1:C:31:GLU:OE2	1:C:86:ARG:HD2	2.20	0.40
1:D:381:ILE:O	1:D:554:ARG:HA	2.21	0.40
1:A:482:GLY:HA2	1:A:483:SER:HB3	2.03	0.40
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.95	0.40
1:C:39:MET:SD	1:C:291:SER:HB3	2.62	0.40
1:D:23:PHE:O	1:D:27:VAL:HG13	2.21	0.40
1:D:491:GLN:O	1:D:495:ILE:HG13	2.21	0.40
1:A:543:LEU:C	1:A:545:THR:H	2.25	0.40
1:A:391:LEU:HD12	1:A:555:LEU:HD13	2.02	0.40
1:B:239:LYS:HB2	1:C:110:TYR:CE1	2.56	0.40
1:B:250:ILE:HG22	1:C:102:LYS:CB	2.49	0.40
1:B:280:LEU:HD22	1:B:280:LEU:HA	1.94	0.40
1:C:172:TYR:HA	1:C:175:THR:HG23	2.03	0.40
1:B:427:TYR:CZ	1:C:223:LYS:HE3	2.57	0.40
1:C:527:ILE:HG23	1:C:536:MET:HE1	2.03	0.40
1:D:180:ILE:HA	1:D:180:ILE:HD13	1.88	0.40
1:D:405:GLN:CD	1:D:407:LEU:HD21	2.41	0.40
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.86	0.40
1:A:23:PHE:O	1:A:23:PHE:HD1	2.05	0.40
1:A:329:GLN:C	1:A:331:LEU:H	2.25	0.40
1:B:111:LYS:CB	1:B:332:ARG:HH22	2.35	0.40
1:B:338:LEU:HD23	1:B:338:LEU:HA	1.87	0.40
1:B:365:PHE:CD1	1:B:368:LEU:HD23	2.57	0.40
1:C:104:ARG:HA	1:C:104:ARG:HD3	1.78	0.40
1:C:119:ILE:HG21	1:C:119:ILE:HD13	1.87	0.40
1:C:143:LEU:O	1:C:147:ILE:HG13	2.21	0.40
1:D:125:THR:HG22	3:D:724:HOH:O	2.22	0.40
1:D:274:ILE:HD13	1:D:274:ILE:HA	1.79	0.40
1:D:527:ILE:HA	1:D:530:ILE:HG12	2.02	0.40
1:B:246:SER:O	1:B:250:ILE:HG23	2.20	0.40
1:C:266:ILE:HA	1:C:266:ILE:HD12	1.74	0.40
1:D:293:ILE:HG21	1:D:293:ILE:HD13	1.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	562/564 (100%)	475 (84%)	58 (10%)	29 (5%)	2	8
1	B	562/564 (100%)	475 (84%)	57 (10%)	30 (5%)	2	7
1	C	562/564 (100%)	473 (84%)	62 (11%)	27 (5%)	2	10
1	D	562/564 (100%)	476 (85%)	57 (10%)	29 (5%)	2	8
All	All	2248/2256 (100%)	1899 (84%)	234 (10%)	115 (5%)	2	8

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	50	TYR
1	A	67	PRO
1	A	282	ASN
1	A	284	SER
1	A	286	ILE
1	A	361	LYS
1	A	366	LYS
1	A	439	ILE
1	A	443	ILE
1	A	447	ASP
1	A	451	GLU
1	A	502	GLU
1	A	543	LEU
1	A	557	HIS
1	B	49	SER
1	B	50	TYR
1	B	67	PRO
1	B	283	GLU
1	B	284	SER
1	B	337	ASN
1	B	355	SER

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Mol	Chain	Res	Type
1	B	361	LYS
1	B	439	ILE
1	B	443	ILE
1	B	447	ASP
1	B	451	GLU
1	B	480	ASP
1	B	502	GLU
1	B	543	LEU
1	B	557	HIS
1	C	49	SER
1	C	283	GLU
1	C	355	SER
1	C	361	LYS
1	C	439	ILE
1	C	443	ILE
1	C	447	ASP
1	C	451	GLU
1	C	480	ASP
1	C	502	GLU
1	C	543	LEU
1	D	49	SER
1	D	50	TYR
1	D	284	SER
1	D	355	SER
1	D	361	LYS
1	D	439	ILE
1	D	443	ILE
1	D	447	ASP
1	D	451	GLU
1	D	480	ASP
1	D	502	GLU
1	D	543	LEU
1	D	557	HIS
1	A	54	ASN
1	A	327	ILE
1	A	337	ASN
1	A	355	SER
1	A	471	PRO
1	B	360	GLY
1	B	366	LYS
1	C	50	TYR
1	C	54	ASN

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Mol	Chain	Res	Type
1	C	67	PRO
1	C	284	SER
1	C	286	ILE
1	C	327	ILE
1	C	337	ASN
1	C	360	GLY
1	C	515	LEU
1	C	557	HIS
1	D	54	ASN
1	D	67	PRO
1	D	286	ILE
1	D	327	ILE
1	D	337	ASN
1	D	360	GLY
1	D	384	SER
1	A	360	GLY
1	B	286	ILE
1	B	544	SER
1	C	366	LYS
1	D	285	ASP
1	D	366	LYS
1	D	399	LEU
1	A	64	LEU
1	A	321	HIS
1	A	384	SER
1	A	399	LEU
1	B	54	ASN
1	B	384	SER
1	C	384	SER
1	C	399	LEU
1	D	430	GLN
1	D	442	ASN
1	A	406	ILE
1	A	544	SER
1	B	321	HIS
1	B	399	LEU
1	B	430	GLN
1	C	430	GLN
1	D	406	ILE
1	A	430	GLN
1	A	513	SER
1	B	330	ASN

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Mol	Chain	Res	Type
1	B	406	ILE
1	B	471	PRO
1	B	513	SER
1	C	406	ILE
1	C	471	PRO
1	D	321	HIS
1	D	471	PRO
1	B	327	ILE
1	D	503	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/505 (100%)	440 (87%)	65 (13%)	5	15
1	B	505/505 (100%)	442 (88%)	63 (12%)	5	16
1	C	505/505 (100%)	445 (88%)	60 (12%)	6	18
1	D	505/505 (100%)	443 (88%)	62 (12%)	5	16
All	All	2020/2020 (100%)	1770 (88%)	250 (12%)	5	16

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	23	PHE
1	A	43	THR
1	A	48	PHE
1	A	53	ARG
1	A	60	LEU
1	A	63	TYR
1	A	66	ILE
1	A	68	VAL
1	A	69	PHE
1	A	79	LEU
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	104	ARG
1	A	115	LYS
1	A	125	THR
1	A	130	SER
1	A	135	SER
1	A	136	ILE
1	A	137	THR
1	A	143	LEU
1	A	144	SER
1	A	148	SER
1	A	152	LEU
1	A	166	LEU
1	A	175	THR
1	A	190	VAL
1	A	203	ARG
1	A	214	ILE
1	A	215	LEU
1	A	219	LEU
1	A	226	LYS
1	A	231	GLU
1	A	241	GLN
1	A	251	THR
1	A	255	VAL
1	A	266	ILE
1	A	274	ILE
1	A	280	LEU
1	A	293	ILE
1	A	298	LEU
1	A	302	ARG
1	A	322	SER
1	A	337	ASN
1	A	351	ILE
1	A	353	ASN
1	A	354	LEU
1	A	362	LYS
1	A	368	LEU
1	A	370	LEU
1	A	373	LYS
1	A	386	CYS
1	A	391	LEU
1	A	398	LEU
1	A	417	ASN

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Mol	Chain	Res	Type
1	A	425	ILE
1	A	432	ILE
1	A	439	ILE
1	A	485	LEU
1	A	489	GLN
1	A	504	GLU
1	A	518	GLN
1	A	535	THR
1	A	543	LEU
1	A	554	ARG
1	A	555	LEU
1	B	3	LYS
1	B	17	LEU
1	B	19	PHE
1	B	23	PHE
1	B	43	THR
1	B	48	PHE
1	B	53	ARG
1	B	57	LEU
1	B	63	TYR
1	B	68	VAL
1	B	88	LEU
1	B	104	ARG
1	B	115	LYS
1	B	125	THR
1	B	130	SER
1	B	136	ILE
1	B	143	LEU
1	B	148	SER
1	B	152	LEU
1	B	166	LEU
1	B	175	THR
1	B	176	LEU
1	B	182	MET
1	B	190	VAL
1	B	203	ARG
1	B	215	LEU
1	B	217	THR
1	B	219	LEU
1	B	226	LYS
1	B	231	GLU
1	B	241	GLN

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Mol	Chain	Res	Type
1	B	250	ILE
1	B	251	THR
1	B	255	VAL
1	B	270	VAL
1	B	280	LEU
1	B	290	LEU
1	B	298	LEU
1	B	302	ARG
1	B	322	SER
1	B	329	GLN
1	B	354	LEU
1	B	355	SER
1	B	368	LEU
1	B	370	LEU
1	B	371	ASN
1	B	373	LYS
1	B	381	ILE
1	B	386	CYS
1	B	391	LEU
1	B	398	LEU
1	B	425	ILE
1	B	432	ILE
1	B	435	PHE
1	B	474	VAL
1	B	485	LEU
1	B	489	GLN
1	B	504	GLU
1	B	518	GLN
1	B	535	THR
1	B	543	LEU
1	B	554	ARG
1	B	564	LYS
1	C	3	LYS
1	C	23	PHE
1	C	43	THR
1	C	48	PHE
1	C	53	ARG
1	C	60	LEU
1	C	63	TYR
1	C	64	LEU
1	C	68	VAL
1	C	69	PHE

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Mol	Chain	Res	Type
1	C	88	LEU
1	C	104	ARG
1	C	115	LYS
1	C	125	THR
1	C	130	SER
1	C	135	SER
1	C	136	ILE
1	C	143	LEU
1	C	148	SER
1	C	152	LEU
1	C	166	LEU
1	C	175	THR
1	C	176	LEU
1	C	183	VAL
1	C	190	VAL
1	C	203	ARG
1	C	215	LEU
1	C	217	THR
1	C	219	LEU
1	C	226	LYS
1	C	241	GLN
1	C	251	THR
1	C	255	VAL
1	C	263	LEU
1	C	266	ILE
1	C	280	LEU
1	C	289	ILE
1	C	290	LEU
1	C	292	THR
1	C	298	LEU
1	C	301	TYR
1	C	302	ARG
1	C	322	SER
1	C	329	GLN
1	C	337	ASN
1	C	354	LEU
1	C	368	LEU
1	C	370	LEU
1	C	373	LYS
1	C	386	CYS
1	C	391	LEU
1	C	398	LEU

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Mol	Chain	Res	Type
1	C	435	PHE
1	C	474	VAL
1	C	485	LEU
1	C	489	GLN
1	C	491	GLN
1	C	512	THR
1	C	535	THR
1	C	543	LEU
1	D	3	LYS
1	D	19	PHE
1	D	23	PHE
1	D	43	THR
1	D	48	PHE
1	D	53	ARG
1	D	58	ILE
1	D	60	LEU
1	D	63	TYR
1	D	64	LEU
1	D	68	VAL
1	D	69	PHE
1	D	88	LEU
1	D	90	ASN
1	D	104	ARG
1	D	130	SER
1	D	136	ILE
1	D	143	LEU
1	D	145	THR
1	D	148	SER
1	D	152	LEU
1	D	157	ILE
1	D	166	LEU
1	D	175	THR
1	D	190	VAL
1	D	203	ARG
1	D	214	ILE
1	D	215	LEU
1	D	217	THR
1	D	219	LEU
1	D	226	LYS
1	D	231	GLU
1	D	241	GLN
1	D	251	THR

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Mol	Chain	Res	Type
1	D	255	VAL
1	D	263	LEU
1	D	266	ILE
1	D	270	VAL
1	D	278	LEU
1	D	280	LEU
1	D	298	LEU
1	D	313	SER
1	D	322	SER
1	D	337	ASN
1	D	353	ASN
1	D	354	LEU
1	D	368	LEU
1	D	370	LEU
1	D	373	LYS
1	D	386	CYS
1	D	391	LEU
1	D	398	LEU
1	D	474	VAL
1	D	485	LEU
1	D	486	SER
1	D	489	GLN
1	D	517	THR
1	D	535	THR
1	D	542	ARG
1	D	543	LEU
1	D	554	ARG
1	D	555	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	A	337	ASN
1	A	489	GLN
1	D	491	GLN

### 5.3.3 RNA ⓘ

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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	1PE	A	601	-	15,15,15	1.16	0	14,14,14	0.67	0
2	1PE	B	601	-	15,15,15	1.06	0	14,14,14	0.57	0
2	1PE	B	602	-	15,15,15	0.93	0	14,14,14	0.44	0
2	1PE	C	601	-	15,15,15	1.06	0	14,14,14	0.69	0
2	1PE	D	601	-	15,15,15	1.04	0	14,14,14	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1PE	A	601	-	-	0/13/13/13	0/0/0/0
2	1PE	B	601	-	-	0/13/13/13	0/0/0/0
2	1PE	B	602	-	-	0/13/13/13	0/0/0/0
2	1PE	C	601	-	-	0/13/13/13	0/0/0/0
2	1PE	D	601	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	1PE	1	0
2	C	601	1PE	1	0
2	D	601	1PE	1	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	564/564 (100%)	-0.24	14 (2%) 58 53	34, 71, 144, 270	0
1	B	564/564 (100%)	-0.18	19 (3%) 46 39	32, 74, 151, 231	0
1	C	564/564 (100%)	-0.24	14 (2%) 58 53	36, 74, 149, 283	0
1	D	564/564 (100%)	-0.09	24 (4%) 36 31	28, 70, 149, 261	0
All	All	2256/2256 (100%)	-0.19	71 (3%) 49 43	28, 72, 150, 283	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	282	ASN	9.5
1	D	284	SER	9.0
1	D	283	GLU	8.8
1	A	282	ASN	7.4
1	A	284	SER	6.6
1	A	288	GLY	6.3
1	D	65	ASN	6.1
1	B	515	LEU	5.9
1	D	290	LEU	5.6
1	D	286	ILE	5.4
1	D	323	SER	4.9
1	C	321	HIS	4.8
1	A	279	VAL	4.7
1	D	533	ASP	4.6
1	D	66	ILE	4.5
1	B	516	ASP	4.5
1	C	518	GLN	4.4
1	D	321	HIS	4.1
1	A	321	HIS	3.9
1	A	465	HIS	3.8
1	D	289	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	287	SER	3.7
1	D	60	LEU	3.7
1	A	286	ILE	3.7
1	D	56	TYR	3.5
1	A	294	SER	3.4
1	D	288	GLY	3.4
1	C	6	PHE	3.4
1	C	517	THR	3.4
1	B	290	LEU	3.3
1	D	62	GLU	3.2
1	B	517	THR	3.2
1	D	63	TYR	3.2
1	B	283	GLU	3.2
1	D	532	LYS	3.1
1	B	52	ASP	3.0
1	D	293	ILE	2.9
1	C	465	HIS	2.7
1	C	522	LYS	2.7
1	B	282	ASN	2.6
1	C	288	GLY	2.6
1	B	51	PHE	2.6
1	B	46	SER	2.5
1	C	523	ILE	2.5
1	C	18	PHE	2.5
1	A	283	GLU	2.4
1	D	69	PHE	2.4
1	B	522	LYS	2.4
1	D	319	TYR	2.4
1	C	328	TYR	2.3
1	B	328	TYR	2.3
1	C	330	ASN	2.3
1	B	285	ASP	2.3
1	C	5	LEU	2.3
1	B	288	GLY	2.3
1	A	291	SER	2.3
1	A	472	GLN	2.3
1	D	451	GLU	2.2
1	B	203	ARG	2.2
1	D	465	HIS	2.1
1	A	280	LEU	2.1
1	D	463	LEU	2.1
1	D	287	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	285	ASP	2.1
1	B	289	ILE	2.1
1	C	290	LEU	2.1
1	A	293	ILE	2.1
1	B	281	LYS	2.0
1	A	285	ASP	2.0
1	B	144	SER	2.0
1	B	69	PHE	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
2	1PE	D	601	16/16	0.88	0.20	0.86	62,65,68,70	0
2	1PE	C	601	16/16	0.87	0.21	0.79	62,63,65,66	0
2	1PE	A	601	16/16	0.92	0.14	-0.37	50,51,53,53	0
2	1PE	B	601	16/16	0.95	0.14	-0.68	45,46,49,50	0
2	1PE	B	602	16/16	0.85	0.11	-	117,119,121,121	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.