



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1X9J  
Title : Structure of butyrate kinase 2 reveals both open- and citrate-induced closed conformations: implications for substrate-induced fit conformational changes  
Authors : Diao, J.S.; Sanders, D.A.; Hasson, M.S.  
Deposited on : 2004-08-21  
Resolution : 3.00 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

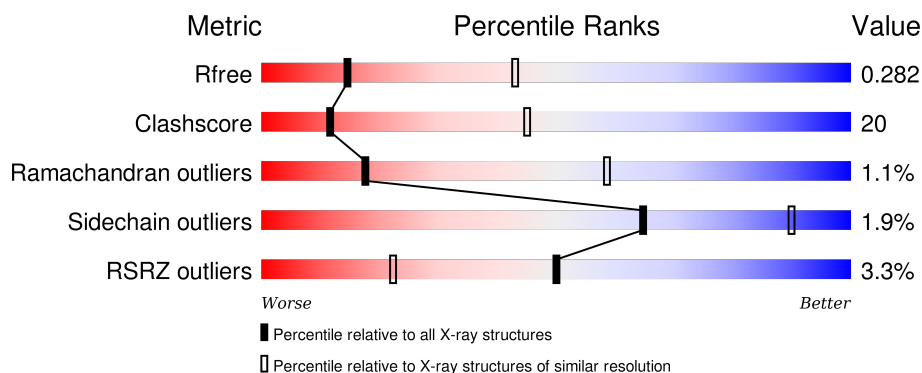
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	375	<div> <div>4%</div> <div>60%</div> <div>38%</div> <div>..</div> </div>
1	B	375	<div> <div>3%</div> <div>59%</div> <div>39%</div> <div>..</div> </div>
1	C	375	<div> <div>3%</div> <div>61%</div> <div>37%</div> <div>..</div> </div>
1	D	375	<div> <div>4%</div> <div>58%</div> <div>40%</div> <div>..</div> </div>
1	E	375	<div> <div>%</div> <div>58%</div> <div>38%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	375	
1	G	375	
1	H	375	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	395	-	X	-	X
5	GOL	B	394	-	X	-	-
5	GOL	C	392	-	X	-	X
5	GOL	D	393	-	X	-	-
5	GOL	F	391	-	X	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23615 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 Probable butyrate kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	B	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	C	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	D	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	E	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	F	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			
1	G	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	H	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

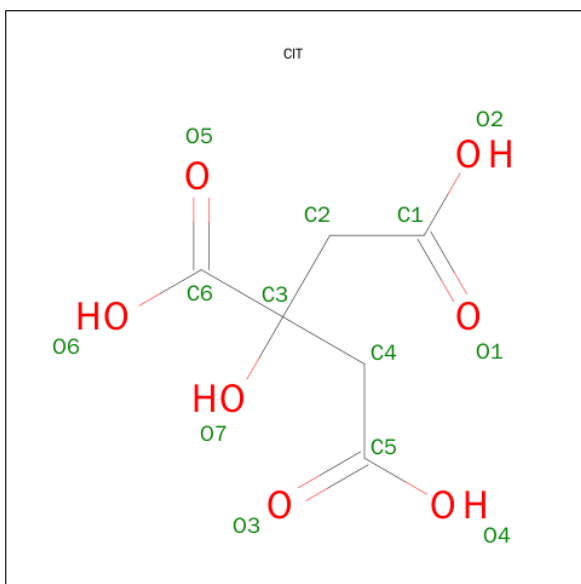
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 13 6 7	0	0
4	G	1	Total C O 13 6 7	0	0
4	G	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0

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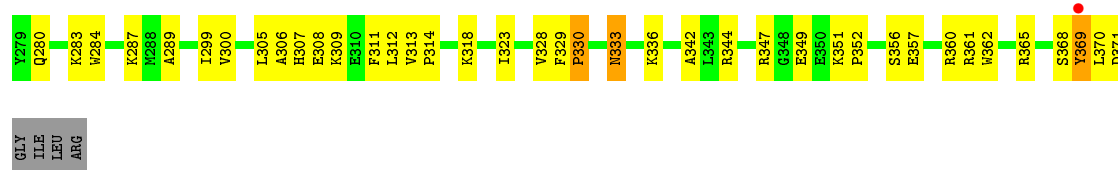
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	7	Total 7	O 7	0	0
6	C	5	Total 5	O 5	0	0
6	D	10	Total 10	O 10	0	0
6	E	4	Total 4	O 4	0	0
6	F	3	Total 3	O 3	0	0
6	G	8	Total 8	O 8	0	0
6	H	2	Total 2	O 2	0	0

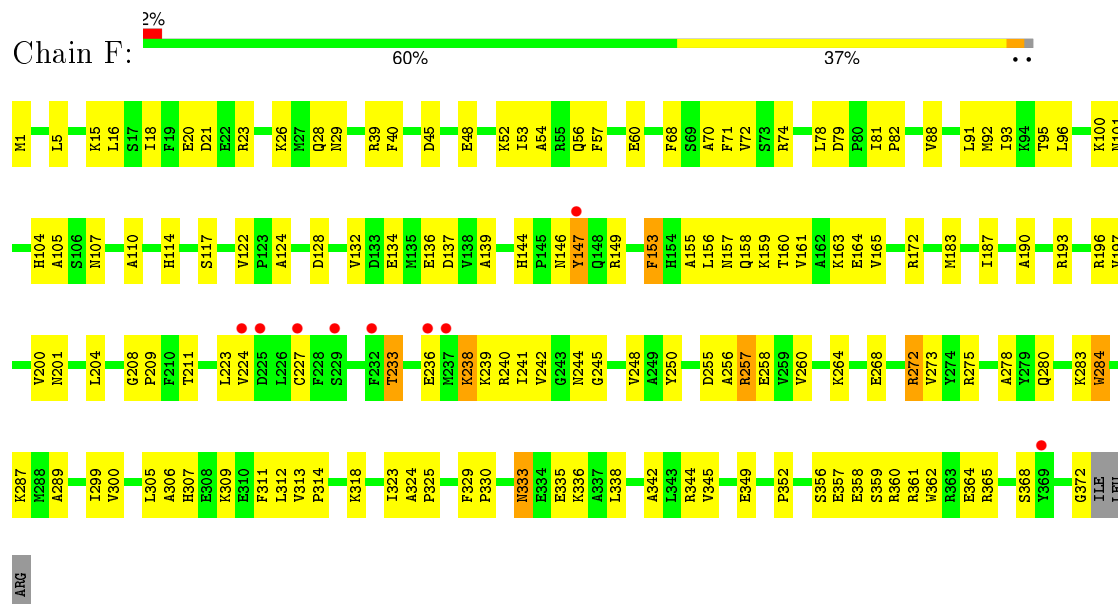




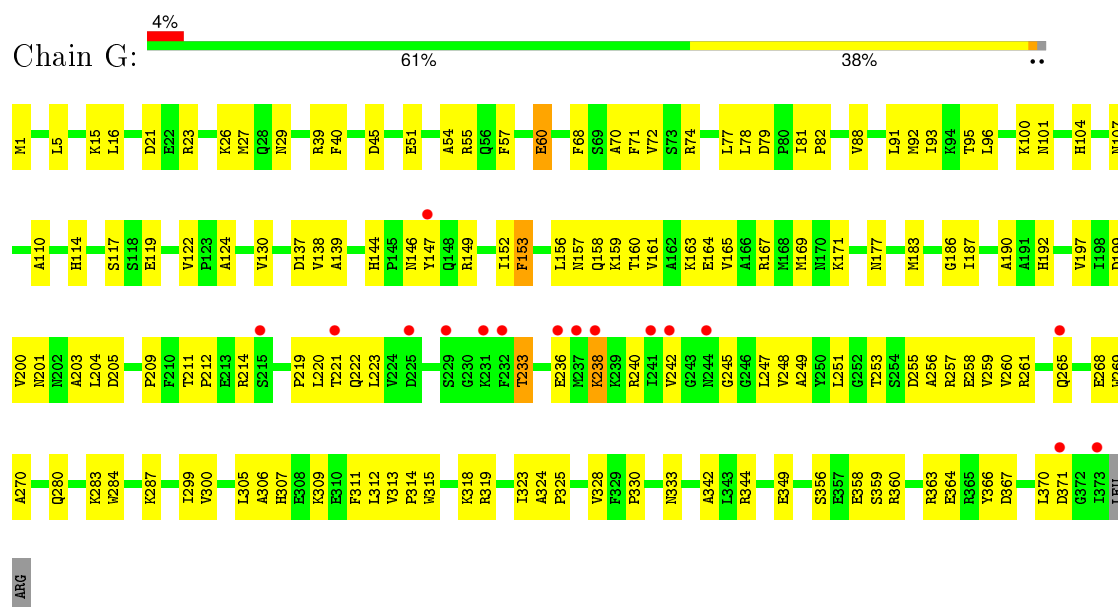




- Molecule 1: Probable butyrate kinase 2

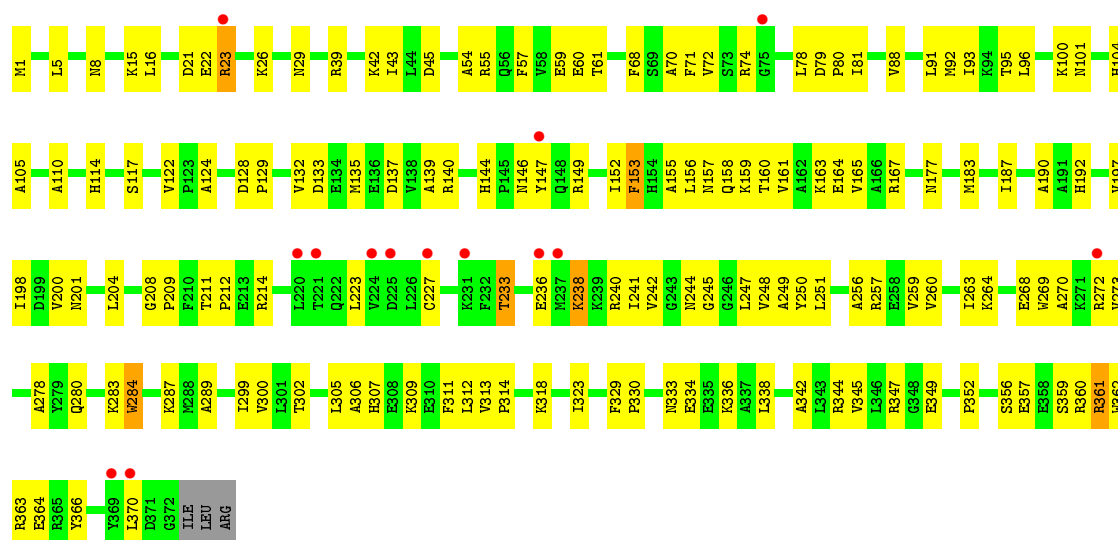


- Molecule 1: Probable butyrate kinase 2



- Molecule 1: Probable butyrate kinase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.68Å 193.68Å 122.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.48 – 3.00 96.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (91.48-3.00) 79.0 (96.84-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.261 , 0.284 0.260 , 0.282	Depositor DCC
$R_{free}$ test set	8832 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 29.4	EDS
Estimated twinning fraction	0.278 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	5 of 98195 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.69 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2748e-04.*

<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: GOL, PO4, CIT, NA

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	0.31	0/2997	0.54	0/4036
1	B	0.30	0/2985	0.55	0/4020
1	C	0.29	0/2985	0.53	0/4020
1	D	0.32	0/2997	0.66	3/4036 (0.1%)
1	E	0.31	0/2985	0.60	3/4020 (0.1%)
1	F	0.33	0/2989	0.67	3/4025 (0.1%)
1	G	0.30	0/2997	0.53	0/4036
1	H	0.31	0/2989	0.62	2/4025 (0.0%)
All	All	0.31	0/23924	0.59	11/32218 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	360	ARG	NE-CZ-NH1	-16.16	112.22	120.30
1	F	272	ARG	NE-CZ-NH1	-15.89	112.35	120.30
1	D	360	ARG	NE-CZ-NH2	15.62	128.11	120.30
1	F	272	ARG	NE-CZ-NH2	15.51	128.05	120.30
1	E	39	ARG	NE-CZ-NH1	-11.90	114.35	120.30
1	H	167	ARG	NE-CZ-NH1	-11.67	114.46	120.30
1	H	167	ARG	NE-CZ-NH2	11.51	126.06	120.30
1	E	39	ARG	NE-CZ-NH2	11.39	126.00	120.30
1	D	360	ARG	CD-NE-CZ	7.32	133.84	123.60
1	F	272	ARG	CD-NE-CZ	7.27	133.78	123.60
1	E	39	ARG	CD-NE-CZ	5.38	131.13	123.60

There are no chirality outliers.

There are no planarity outliers.

## 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	2939	0	2969	119	0
1	B	2927	0	2955	132	0
1	C	2927	0	2955	128	0
1	D	2939	0	2969	136	0
1	E	2927	0	2955	139	0
1	F	2931	0	2958	123	0
1	G	2939	0	2969	126	0
1	H	2931	0	2958	134	0
2	D	1	0	0	0	0
3	B	5	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	D	26	0	10	3	0
4	G	26	0	10	0	0
5	A	6	0	4	0	0
5	B	6	0	4	0	0
5	C	6	0	4	0	0
5	D	6	0	4	0	0
5	F	6	0	4	0	0
6	A	8	0	0	1	0
6	B	7	0	0	1	0
6	C	5	0	0	0	0
6	D	10	0	0	0	0
6	E	4	0	0	0	0
6	F	3	0	0	0	0
6	G	8	0	0	0	0
6	H	2	0	0	0	0
All	All	23615	0	23728	962	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 20.

All (962) 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:88:VAL:HG12	1:A:93:ILE:HD11	1.43	1.00
1:A:257:ARG:HH11	1:A:257:ARG:HB3	1.35	0.91
1:D:88:VAL:HG12	1:D:93:ILE:HD11	1.53	0.90
1:H:344:ARG:HG3	1:H:349:GLU:HB2	1.53	0.90
1:B:88:VAL:HG12	1:B:93:ILE:HD11	1.55	0.89
1:E:344:ARG:HG3	1:E:349:GLU:HB2	1.55	0.89
1:G:88:VAL:HG12	1:G:93:ILE:HD11	1.52	0.88
1:A:344:ARG:HG3	1:A:349:GLU:HB2	1.54	0.88
1:G:344:ARG:HG3	1:G:349:GLU:HB2	1.53	0.87
1:D:344:ARG:HG3	1:D:349:GLU:HB2	1.54	0.87
1:F:272:ARG:HD2	1:G:137:ASP:OD2	1.75	0.86
1:C:333:ASN:ND2	1:C:336:LYS:HB2	1.90	0.85
1:E:261:ARG:NH1	1:E:261:ARG:HB2	1.93	0.84
1:C:196:ARG:HH22	1:C:365:ARG:HH12	1.25	0.82
1:C:309:LYS:NZ	1:D:167:ARG:HD2	1.95	0.81
1:E:261:ARG:HH11	1:E:261:ARG:HB2	1.46	0.81
1:D:72:VAL:HG21	1:D:342:ALA:HB2	1.61	0.81
1:A:72:VAL:HG21	1:A:342:ALA:HB2	1.60	0.81
1:B:72:VAL:HG21	1:B:342:ALA:HB2	1.63	0.81
1:G:167:ARG:HD2	1:H:309:LYS:NZ	1.97	0.80
1:E:306:ALA:HB3	1:E:330:PRO:HA	1.64	0.79
1:A:241:ILE:HG13	1:A:242:VAL:HG23	1.65	0.79
1:B:283:LYS:HE2	1:C:287:LYS:HE2	1.65	0.79
1:C:344:ARG:HG3	1:C:349:GLU:HB2	1.65	0.78
1:B:129:PRO:O	1:B:132:VAL:HG23	1.84	0.78
1:G:72:VAL:HG21	1:G:342:ALA:HB2	1.66	0.78
1:C:196:ARG:NH2	1:C:365:ARG:HH12	1.82	0.78
1:H:72:VAL:HG21	1:H:342:ALA:HB2	1.66	0.78
1:H:137:ASP:O	1:H:140:ARG:HG3	1.83	0.77
1:D:287:LYS:HE2	1:E:283:LYS:HE2	1.66	0.77
1:F:283:LYS:HE2	1:G:287:LYS:HE2	1.66	0.77
1:G:261:ARG:HH11	1:G:261:ARG:HB3	1.48	0.76
1:B:333:ASN:HD22	1:B:336:LYS:HB2	1.51	0.76
1:H:92:MET:HG2	1:H:92:MET:O	1.86	0.76
1:G:360:ARG:O	1:G:363:ARG:HG2	1.84	0.76
1:C:23:ARG:HD2	1:D:257:ARG:HH21	1.49	0.75
1:D:82:PRO:HD2	1:D:358:GLU:HG3	1.68	0.75
1:B:257:ARG:HH21	1:B:257:ARG:HA	1.51	0.75
1:B:241:ILE:HD11	1:C:224:VAL:HG21	1.67	0.75
1:D:77:LEU:HD21	1:D:204:LEU:CD1	2.17	0.75
1:E:240:ARG:HA	1:E:244:ASN:OD1	1.88	0.74
1:C:26:LYS:HE2	1:C:57:PHE:CE1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:LYS:HE2	1:G:57:PHE:CE1	2.22	0.74
1:G:214:ARG:HE	1:G:242:VAL:HG13	1.53	0.74
1:F:72:VAL:HG21	1:F:342:ALA:HB2	1.69	0.74
1:A:27:MET:HG2	1:B:24:MET:HE3	1.70	0.74
1:D:283:LYS:HE2	1:E:287:LYS:HE2	1.70	0.74
1:B:287:LYS:HE2	1:C:283:LYS:HE2	1.68	0.73
1:A:287:LYS:HE2	1:H:283:LYS:HE2	1.71	0.72
1:G:261:ARG:NH1	1:G:261:ARG:HB3	2.03	0.72
1:B:26:LYS:HE2	1:B:57:PHE:CE1	2.24	0.72
1:D:261:ARG:HG2	1:D:265:GLN:HE21	1.53	0.71
1:E:245:GLY:O	1:E:248:VAL:HG12	1.90	0.71
1:A:283:LYS:HE2	1:H:287:LYS:HE2	1.72	0.71
1:B:251:LEU:HD21	1:B:270:ALA:HA	1.71	0.71
1:B:82:PRO:HD2	1:B:358:GLU:HG3	1.72	0.71
1:C:72:VAL:HG21	1:C:342:ALA:HB2	1.73	0.70
1:E:72:VAL:HG21	1:E:342:ALA:HB2	1.73	0.70
1:E:365:ARG:O	1:E:369:TYR:HB2	1.91	0.70
1:E:26:LYS:HE2	1:E:57:PHE:CE1	2.27	0.70
1:E:91:LEU:HD23	1:E:356:SER:HA	1.74	0.70
1:G:167:ARG:HD2	1:H:309:LYS:CE	2.21	0.70
1:H:88:VAL:HG12	1:H:93:ILE:HD11	1.73	0.70
1:E:255:ASP:OD1	1:E:257:ARG:HG3	1.92	0.69
1:E:261:ARG:HG2	1:E:265:GLN:HE21	1.57	0.69
1:F:287:LYS:HE2	1:G:283:LYS:HE2	1.74	0.69
1:D:88:VAL:CG1	1:D:93:ILE:HD11	2.22	0.69
1:D:208:GLY:HA2	1:D:284:TRP:CZ2	2.27	0.69
1:H:359:SER:O	1:H:363:ARG:HG3	1.93	0.69
1:C:333:ASN:HD22	1:C:336:LYS:HB2	1.57	0.69
1:D:256:ALA:O	1:D:260:VAL:HG23	1.94	0.68
1:B:259:VAL:O	1:B:263:ILE:HG13	1.94	0.68
1:H:360:ARG:O	1:H:364:GLU:HG3	1.94	0.68
1:E:240:ARG:HD2	1:E:244:ASN:ND2	2.08	0.67
1:D:220:LEU:HD22	1:E:223:LEU:HD22	1.75	0.67
1:C:309:LYS:CE	1:D:167:ARG:HD2	2.23	0.67
1:H:208:GLY:HA2	1:H:284:TRP:CZ2	2.29	0.67
1:A:257:ARG:NH1	1:A:257:ARG:HB3	2.10	0.67
1:F:245:GLY:O	1:F:248:VAL:HG12	1.95	0.67
1:H:250:TYR:HB3	1:H:273:VAL:HG21	1.76	0.67
1:G:248:VAL:HA	1:G:253:THR:O	1.93	0.67
1:G:167:ARG:HD2	1:H:309:LYS:HZ1	1.59	0.67
1:D:129:PRO:O	1:D:132:VAL:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:LEU:HD21	1:G:204:LEU:CD1	2.24	0.66
1:C:240:ARG:HD2	1:C:244:ASN:HD21	1.59	0.66
1:E:144:HIS:CE1	1:E:146:ASN:HD22	2.14	0.66
1:E:208:GLY:HA2	1:E:284:TRP:CZ2	2.29	0.66
1:C:23:ARG:HD2	1:D:257:ARG:NH2	2.11	0.66
1:C:240:ARG:HD2	1:C:244:ASN:ND2	2.10	0.66
1:E:369:TYR:HB3	1:E:370:LEU:HD12	1.77	0.65
1:A:241:ILE:HG13	1:A:242:VAL:H	1.61	0.65
1:A:360:ARG:O	1:A:364:GLU:HG3	1.96	0.65
1:G:167:ARG:HD2	1:H:309:LYS:HE2	1.76	0.65
1:E:328:VAL:HG12	1:E:330:PRO:HD3	1.77	0.65
1:H:23:ARG:H	1:H:23:ARG:HD2	1.60	0.65
1:B:306:ALA:HB3	1:B:330:PRO:HA	1.78	0.65
1:E:161:VAL:O	1:E:165:VAL:HG23	1.97	0.65
1:H:214:ARG:HE	1:H:242:VAL:HG23	1.61	0.65
1:E:214:ARG:NE	1:E:242:VAL:HG23	2.12	0.65
1:H:256:ALA:O	1:H:260:VAL:HG23	1.96	0.65
1:G:256:ALA:O	1:G:260:VAL:HG23	1.96	0.65
1:D:356:SER:HB3	1:D:360:ARG:NH1	2.12	0.64
1:D:306:ALA:HB3	1:D:330:PRO:HA	1.79	0.64
1:H:55:ARG:HH11	1:H:55:ARG:HG2	1.63	0.64
1:G:91:LEU:HD23	1:G:356:SER:HA	1.80	0.64
1:A:72:VAL:HG21	1:A:342:ALA:CB	2.26	0.64
1:E:128:ASP:HB2	1:E:156:LEU:HA	1.79	0.64
1:F:190:ALA:HB1	1:F:197:VAL:HG13	1.78	0.64
1:B:361:ARG:O	1:B:365:ARG:HG3	1.97	0.64
1:A:241:ILE:HG13	1:A:242:VAL:N	2.13	0.64
1:G:212:PRO:HA	1:G:247:LEU:HB2	1.79	0.64
1:C:258:GLU:O	1:C:261:ARG:HB3	1.98	0.64
1:E:135:MET:HA	1:E:198:ILE:HA	1.79	0.64
1:H:214:ARG:NE	1:H:242:VAL:HG23	2.12	0.64
1:F:161:VAL:O	1:F:165:VAL:HG23	1.97	0.64
1:H:135:MET:HA	1:H:198:ILE:HA	1.80	0.63
1:G:130:VAL:HG23	1:G:153:PHE:O	1.96	0.63
1:A:91:LEU:HD23	1:A:356:SER:HA	1.79	0.63
1:A:219:PRO:HG2	1:A:222:GLN:NE2	2.13	0.63
1:H:313:VAL:HB	1:H:314:PRO:HD3	1.80	0.63
1:A:258:GLU:O	1:A:261:ARG:HB3	1.98	0.63
1:F:313:VAL:HB	1:F:314:PRO:HD3	1.81	0.63
1:D:255:ASP:O	1:D:259:VAL:HG23	1.99	0.63
1:A:240:ARG:HH21	1:H:144:HIS:CE1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:ARG:O	1:G:364:GLU:HG3	1.98	0.63
1:D:43:ILE:HD12	1:D:103:GLU:HB3	1.80	0.63
1:H:212:PRO:HA	1:H:247:LEU:HB3	1.80	0.63
1:C:309:LYS:HE2	1:D:167:ARG:HD2	1.79	0.62
1:C:144:HIS:CE1	1:C:146:ASN:HD22	2.17	0.62
1:D:313:VAL:HB	1:D:314:PRO:HD3	1.81	0.62
1:H:26:LYS:HE2	1:H:57:PHE:CE1	2.35	0.62
1:D:161:VAL:O	1:D:165:VAL:HG23	1.99	0.62
1:D:72:VAL:HG21	1:D:342:ALA:CB	2.30	0.62
1:H:95:THR:HG23	1:H:100:LYS:HD3	1.82	0.62
1:H:161:VAL:O	1:H:165:VAL:HG23	2.00	0.62
1:F:240:ARG:NH1	1:F:244:ASN:HD21	1.98	0.62
1:B:161:VAL:O	1:B:165:VAL:HG23	2.00	0.61
1:G:82:PRO:HD2	1:G:358:GLU:HG3	1.81	0.61
1:G:81:ILE:HG22	1:G:359:SER:HA	1.82	0.61
1:B:93:ILE:H	1:B:93:ILE:HD12	1.65	0.61
1:G:360:ARG:HA	1:G:363:ARG:NE	2.15	0.61
1:D:95:THR:HG23	1:D:100:LYS:HD3	1.83	0.61
1:G:161:VAL:O	1:G:165:VAL:HG23	1.99	0.61
1:A:95:THR:HG23	1:A:100:LYS:HD3	1.82	0.61
1:B:95:THR:HG23	1:B:100:LYS:HD3	1.83	0.61
1:B:81:ILE:HG22	1:B:359:SER:HA	1.82	0.61
1:E:238:LYS:HB2	1:E:238:LYS:NZ	2.15	0.61
1:F:157:ASN:ND2	1:F:161:VAL:HG13	2.16	0.61
1:C:95:THR:HG23	1:C:100:LYS:HD3	1.81	0.61
1:E:356:SER:HB3	1:E:360:ARG:HH12	1.65	0.61
1:H:356:SER:HB3	1:H:360:ARG:HH12	1.66	0.61
1:C:161:VAL:O	1:C:165:VAL:HG23	2.01	0.61
1:E:313:VAL:HB	1:E:314:PRO:HD3	1.83	0.61
1:H:238:LYS:HB2	1:H:238:LYS:NZ	2.16	0.61
1:A:161:VAL:O	1:A:165:VAL:HG23	2.01	0.60
1:C:238:LYS:HB2	1:C:238:LYS:NZ	2.15	0.60
1:D:238:LYS:NZ	1:D:238:LYS:HB2	2.16	0.60
1:G:313:VAL:HB	1:G:314:PRO:HD3	1.82	0.60
1:H:157:ASN:ND2	1:H:161:VAL:HG13	2.16	0.60
1:F:95:THR:HG23	1:F:100:LYS:HD3	1.82	0.60
1:G:95:THR:HG23	1:G:100:LYS:HD3	1.83	0.60
1:D:81:ILE:HG22	1:D:359:SER:HA	1.82	0.60
1:B:313:VAL:HB	1:B:314:PRO:HD3	1.83	0.60
1:A:238:LYS:HB2	1:A:238:LYS:NZ	2.15	0.60
1:E:157:ASN:ND2	1:E:161:VAL:HG13	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:PHE:HB3	1:C:45:ASP:HB2	1.82	0.60
1:E:248:VAL:HA	1:E:253:THR:O	2.02	0.60
1:E:251:LEU:HD21	1:E:270:ALA:HA	1.83	0.60
1:G:238:LYS:HB2	1:G:238:LYS:NZ	2.16	0.60
1:B:238:LYS:HB2	1:B:238:LYS:NZ	2.17	0.60
1:A:313:VAL:HB	1:A:314:PRO:HD3	1.83	0.60
1:D:93:ILE:O	1:D:93:ILE:HG22	2.00	0.60
1:D:220:LEU:HD12	1:E:241:ILE:HG23	1.83	0.60
1:E:261:ARG:HH11	1:E:261:ARG:CB	2.13	0.60
1:B:157:ASN:ND2	1:B:161:VAL:HG13	2.17	0.60
1:E:95:THR:HG23	1:E:100:LYS:HD3	1.83	0.60
1:D:219:PRO:HG2	1:D:222:GLN:NE2	2.16	0.60
1:D:134:GLU:OE2	1:D:196:ARG:HA	2.02	0.59
1:G:356:SER:HB3	1:G:360:ARG:HH12	1.68	0.59
1:C:144:HIS:CE1	1:C:146:ASN:ND2	2.70	0.59
1:B:144:HIS:CE1	1:C:240:ARG:HH21	2.21	0.59
1:B:356:SER:HB3	1:B:360:ARG:HH12	1.67	0.59
1:F:238:LYS:NZ	1:F:238:LYS:HB2	2.16	0.59
1:F:92:MET:HG2	1:F:92:MET:O	2.02	0.59
1:F:128:ASP:HB2	1:F:156:LEU:HA	1.84	0.59
1:B:257:ARG:HH21	1:B:257:ARG:CA	2.15	0.59
1:G:214:ARG:NE	1:G:242:VAL:HG13	2.16	0.59
1:B:36:GLU:OE1	1:B:49:PHE:HZ	1.86	0.59
1:H:79:ASP:HB2	1:H:363:ARG:NH1	2.18	0.58
1:C:313:VAL:HB	1:C:314:PRO:HD3	1.84	0.58
1:H:259:VAL:O	1:H:263:ILE:HG13	2.04	0.58
1:H:251:LEU:HD21	1:H:270:ALA:HA	1.85	0.58
1:B:333:ASN:ND2	1:B:336:LYS:H	2.00	0.58
1:E:214:ARG:HE	1:E:242:VAL:HG23	1.68	0.58
1:F:333:ASN:HB3	1:F:336:LYS:HB3	1.85	0.58
1:A:26:LYS:HE2	1:A:57:PHE:CE1	2.38	0.58
1:C:91:LEU:HD23	1:C:356:SER:HA	1.86	0.58
1:B:248:VAL:HG13	1:B:249:ALA:N	2.18	0.58
1:F:356:SER:HB3	1:F:360:ARG:HH12	1.67	0.58
1:B:36:GLU:OE1	1:B:49:PHE:CZ	2.57	0.58
1:F:255:ASP:OD1	1:F:257:ARG:HB2	2.03	0.58
1:G:187:ILE:HG13	1:G:211:THR:HG22	1.86	0.57
1:D:258:GLU:HA	1:D:261:ARG:NH1	2.19	0.57
1:D:91:LEU:HD23	1:D:356:SER:HA	1.86	0.57
1:C:356:SER:HB3	1:C:360:ARG:HH12	1.68	0.57
1:C:309:LYS:HZ1	1:D:167:ARG:HD2	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ASN:HB3	1:E:284:TRP:CZ3	2.38	0.57
1:A:157:ASN:ND2	1:A:161:VAL:HG13	2.18	0.57
1:H:240:ARG:HA	1:H:244:ASN:HB2	1.85	0.57
1:C:157:ASN:ND2	1:C:161:VAL:HG13	2.19	0.57
1:B:91:LEU:HD23	1:B:356:SER:HA	1.85	0.57
1:C:60:GLU:OE2	1:D:60:GLU:HB3	2.05	0.57
1:H:302:THR:HA	1:H:329:PHE:O	2.05	0.57
1:B:70:ALA:HA	1:B:122:VAL:HG12	1.87	0.57
1:B:72:VAL:HG21	1:B:342:ALA:CB	2.34	0.57
1:D:154:HIS:NE2	4:D:381:CIT:H41	2.20	0.57
1:C:306:ALA:HB3	1:C:330:PRO:HA	1.85	0.57
1:D:239:LYS:O	1:D:244:ASN:HB3	2.05	0.57
1:F:147:TYR:N	1:F:147:TYR:CD1	2.73	0.57
1:D:157:ASN:ND2	1:D:161:VAL:HG13	2.19	0.56
1:H:245:GLY:O	1:H:248:VAL:HG12	2.05	0.56
1:B:40:PHE:HB3	1:B:45:ASP:HB2	1.86	0.56
1:D:160:THR:O	1:D:164:GLU:HG3	2.05	0.56
1:A:24:MET:HE3	1:B:27:MET:HG2	1.86	0.56
1:A:27:MET:HG2	1:B:24:MET:CE	2.36	0.56
1:C:240:ARG:HH11	1:C:244:ASN:ND2	2.03	0.56
1:A:356:SER:HB3	1:A:360:ARG:HH12	1.70	0.56
1:C:261:ARG:HG2	1:C:265:GLN:HE21	1.71	0.56
1:C:135:MET:HA	1:C:198:ILE:HA	1.86	0.56
1:B:272:ARG:HD2	1:C:369:TYR:CE1	2.40	0.56
1:D:223:LEU:HD21	1:E:224:VAL:CG2	2.36	0.56
1:C:144:HIS:HE1	1:C:146:ASN:ND2	2.03	0.56
1:D:26:LYS:HE2	1:D:57:PHE:CE1	2.41	0.56
1:F:139:ALA:O	1:F:149:ARG:HD3	2.05	0.56
1:G:72:VAL:HG21	1:G:342:ALA:CB	2.36	0.56
1:G:139:ALA:O	1:G:149:ARG:HD3	2.05	0.56
1:B:104:HIS:CD2	1:B:105:ALA:H	2.24	0.56
1:H:74:ARG:HH11	1:H:74:ARG:HG2	1.71	0.56
1:E:240:ARG:HA	1:E:244:ASN:ND2	2.21	0.56
1:G:157:ASN:ND2	1:G:161:VAL:HG13	2.19	0.56
1:F:344:ARG:HG3	1:F:349:GLU:HB2	1.87	0.56
1:A:139:ALA:O	1:A:149:ARG:HD3	2.06	0.56
1:B:160:THR:O	1:B:164:GLU:HG3	2.06	0.56
1:C:74:ARG:HG2	1:C:74:ARG:HH11	1.70	0.56
1:D:259:VAL:O	1:D:263:ILE:HG13	2.06	0.56
1:F:160:THR:O	1:F:164:GLU:HG3	2.06	0.56
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:THR:O	1:G:164:GLU:HG3	2.06	0.56
1:B:357:GLU:O	1:B:361:ARG:HG3	2.06	0.56
1:E:139:ALA:O	1:E:149:ARG:HD3	2.06	0.56
1:F:91:LEU:HD23	1:F:356:SER:HA	1.88	0.55
1:G:190:ALA:HB1	1:G:197:VAL:HG13	1.88	0.55
1:B:148:GLN:HG3	1:B:366:TYR:OH	2.06	0.55
1:F:70:ALA:HA	1:F:122:VAL:HG12	1.88	0.55
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.71	0.55
1:E:74:ARG:HG2	1:E:74:ARG:HH11	1.71	0.55
1:A:70:ALA:HA	1:A:122:VAL:HG12	1.88	0.55
1:G:255:ASP:HB3	1:G:258:GLU:CB	2.36	0.55
1:E:219:PRO:HG2	1:E:222:GLN:NE2	2.22	0.55
1:C:160:THR:O	1:C:164:GLU:HG3	2.06	0.55
1:B:139:ALA:O	1:B:149:ARG:HD3	2.06	0.55
1:B:80:PRO:HB2	1:B:362:TRP:CE3	2.41	0.55
1:H:160:THR:O	1:H:164:GLU:HG3	2.07	0.55
1:H:70:ALA:HA	1:H:122:VAL:HG12	1.89	0.55
1:F:239:LYS:O	1:F:244:ASN:HB3	2.06	0.55
1:C:190:ALA:HB1	1:C:197:VAL:HG13	1.89	0.55
1:D:187:ILE:HG13	1:D:211:THR:HG22	1.89	0.55
1:H:139:ALA:O	1:H:149:ARG:HD3	2.07	0.55
1:H:43:ILE:C	1:H:45:ASP:H	2.10	0.55
1:F:114:HIS:O	1:F:117:SER:HB3	2.07	0.55
1:A:245:GLY:O	1:A:248:VAL:HG12	2.07	0.55
1:A:114:HIS:O	1:A:117:SER:HB3	2.07	0.54
1:F:40:PHE:HB3	1:F:45:ASP:HB2	1.90	0.54
1:B:5:LEU:HB2	1:B:68:PHE:CE2	2.42	0.54
1:D:40:PHE:HB3	1:D:45:ASP:HB2	1.88	0.54
1:C:153:PHE:CD1	1:C:158:GLN:HG3	2.43	0.54
1:E:240:ARG:HA	1:E:244:ASN:CG	2.27	0.54
1:D:190:ALA:HB1	1:D:197:VAL:HG13	1.89	0.54
1:F:257:ARG:HB3	1:F:257:ARG:NH1	2.23	0.54
1:F:223:LEU:HD22	1:G:220:LEU:HD22	1.89	0.54
1:D:70:ALA:HA	1:D:122:VAL:HG12	1.89	0.54
1:D:212:PRO:O	1:D:248:VAL:HG23	2.08	0.54
1:A:88:VAL:HG12	1:A:93:ILE:CD1	2.29	0.54
1:E:40:PHE:HB3	1:E:45:ASP:HB2	1.90	0.54
1:D:241:ILE:HD13	1:E:220:LEU:HB3	1.90	0.54
1:D:223:LEU:HD23	1:E:223:LEU:HD23	1.89	0.54
1:B:268:GLU:HG3	1:C:369:TYR:OH	2.07	0.54
1:E:52:LYS:O	1:E:56:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLU:OE1	1:C:261:ARG:HD2	2.08	0.54
1:H:240:ARG:NH1	1:H:244:ASN:HB3	2.23	0.54
1:C:328:VAL:HG12	1:C:330:PRO:HD3	1.90	0.54
1:G:261:ARG:O	1:G:265:GLN:HG3	2.08	0.54
1:H:79:ASP:CB	1:H:363:ARG:NH1	2.71	0.54
1:H:91:LEU:HD23	1:H:356:SER:HA	1.90	0.53
1:G:70:ALA:HA	1:G:122:VAL:HG12	1.90	0.53
1:C:344:ARG:CG	1:C:349:GLU:HB2	2.37	0.53
1:G:153:PHE:CD1	1:G:158:GLN:HG3	2.43	0.53
1:B:333:ASN:HD22	1:B:336:LYS:CB	2.21	0.53
1:D:82:PRO:CD	1:D:358:GLU:HG3	2.36	0.53
1:A:24:MET:HE3	1:B:24:MET:HE3	1.91	0.53
1:F:257:ARG:HA	1:F:257:ARG:CZ	2.39	0.53
1:E:144:HIS:HE1	1:E:146:ASN:HD22	1.54	0.53
1:C:5:LEU:HB2	1:C:68:PHE:CE2	2.44	0.53
1:H:306:ALA:HB3	1:H:330:PRO:HA	1.89	0.53
1:F:74:ARG:HG2	1:F:74:ARG:HH11	1.74	0.53
1:G:245:GLY:HA2	1:G:249:ALA:HB2	1.91	0.53
1:F:147:TYR:HD1	1:F:147:TYR:H	1.56	0.53
1:A:223:LEU:HD23	1:H:223:LEU:HD23	1.91	0.53
1:B:248:VAL:HG13	1:B:249:ALA:H	1.73	0.53
1:C:139:ALA:O	1:C:149:ARG:HD3	2.09	0.53
1:C:241:ILE:HG13	1:C:242:VAL:HG13	1.90	0.53
1:H:42:LYS:O	1:H:45:ASP:HB2	2.08	0.53
1:F:72:VAL:HG21	1:F:342:ALA:CB	2.37	0.53
1:D:39:ARG:HB3	1:D:40:PHE:CE1	2.44	0.53
1:G:74:ARG:HH11	1:G:74:ARG:HG2	1.73	0.53
1:A:248:VAL:O	1:A:252:GLY:HA2	2.09	0.53
1:F:256:ALA:O	1:F:260:VAL:HG23	2.09	0.53
1:F:26:LYS:HE2	1:F:57:PHE:CE1	2.43	0.53
1:F:187:ILE:HG13	1:F:211:THR:HG22	1.91	0.53
1:F:153:PHE:CD1	1:F:158:GLN:HG3	2.43	0.53
1:H:187:ILE:HG13	1:H:211:THR:HG22	1.90	0.53
1:G:255:ASP:HB3	1:G:258:GLU:HB3	1.91	0.53
1:A:40:PHE:HB3	1:A:45:ASP:HB2	1.90	0.53
1:G:23:ARG:HG3	1:G:23:ARG:HH11	1.74	0.53
1:D:74:ARG:HG2	1:D:74:ARG:HH11	1.73	0.52
1:E:240:ARG:HD2	1:E:244:ASN:HD21	1.71	0.52
1:F:223:LEU:HD23	1:G:223:LEU:HD23	1.91	0.52
1:A:140:ARG:NH1	1:A:365:ARG:HH12	2.07	0.52
1:C:70:ALA:HA	1:C:122:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PRO:HG2	1:C:222:GLN:NE2	2.24	0.52
1:C:114:HIS:O	1:C:117:SER:HB3	2.09	0.52
1:C:22:GLU:OE2	1:C:347:ARG:NH2	2.41	0.52
1:A:153:PHE:CD1	1:A:158:GLN:HG3	2.44	0.52
1:A:160:THR:O	1:A:164:GLU:HG3	2.09	0.52
1:E:92:MET:HG2	1:E:92:MET:O	2.08	0.52
1:B:114:HIS:O	1:B:117:SER:HB3	2.09	0.52
1:D:5:LEU:HB2	1:D:68:PHE:CE2	2.43	0.52
1:H:153:PHE:CD1	1:H:158:GLN:HG3	2.45	0.52
1:D:139:ALA:O	1:D:149:ARG:HD3	2.09	0.52
1:G:255:ASP:O	1:G:259:VAL:HG23	2.09	0.52
1:G:153:PHE:HD1	1:G:158:GLN:HG3	1.75	0.52
1:B:256:ALA:O	1:B:260:VAL:HG23	2.10	0.52
1:B:187:ILE:HG13	1:B:211:THR:HG22	1.91	0.52
1:B:190:ALA:HB1	1:B:197:VAL:HG13	1.91	0.52
1:E:368:SER:HA	1:E:371:ASP:HB3	1.91	0.52
1:C:257:ARG:NH1	1:C:308:GLU:HG2	2.25	0.52
1:C:257:ARG:HH12	1:C:308:GLU:HA	1.75	0.52
1:A:209:PRO:HD3	1:A:284:TRP:CD2	2.45	0.52
1:E:88:VAL:HG12	1:E:93:ILE:HD11	1.92	0.52
1:A:187:ILE:HG13	1:A:211:THR:HG22	1.91	0.52
1:G:5:LEU:HB2	1:G:68:PHE:CE2	2.44	0.52
1:E:153:PHE:CD1	1:E:158:GLN:HG3	2.44	0.52
1:B:82:PRO:CD	1:B:358:GLU:HG3	2.40	0.52
1:F:241:ILE:HD13	1:G:220:LEU:HB3	1.91	0.52
1:F:18:ILE:HG13	1:F:57:PHE:HE2	1.75	0.52
1:H:114:HIS:O	1:H:117:SER:HB3	2.10	0.51
1:G:280:GLN:O	1:G:284:TRP:HE3	1.93	0.51
1:D:153:PHE:CD1	1:D:158:GLN:HG3	2.45	0.51
1:C:152:ILE:HG21	1:C:204:LEU:HD12	1.92	0.51
1:F:5:LEU:HB2	1:F:68:PHE:CE2	2.46	0.51
1:H:190:ALA:HB1	1:H:197:VAL:HG13	1.91	0.51
1:A:5:LEU:HB2	1:A:68:PHE:CE2	2.46	0.51
1:H:251:LEU:CD2	1:H:270:ALA:HA	2.40	0.51
1:C:81:ILE:O	1:C:132:VAL:HA	2.10	0.51
1:G:40:PHE:HB3	1:G:45:ASP:HB2	1.91	0.51
1:C:259:VAL:O	1:C:263:ILE:HG13	2.10	0.51
1:E:114:HIS:O	1:E:117:SER:HB3	2.10	0.51
1:G:261:ARG:CB	1:G:261:ARG:HH11	2.19	0.51
1:H:344:ARG:CG	1:H:349:GLU:HB2	2.35	0.51
1:E:18:ILE:HG13	1:E:57:PHE:HE2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:ARG:HA	1:F:244:ASN:HB3	1.92	0.51
1:F:153:PHE:HD1	1:F:158:GLN:HG3	1.74	0.51
1:H:59:GLU:C	1:H:61:THR:H	2.13	0.51
1:C:247:LEU:HD23	1:C:273:VAL:HG12	1.92	0.51
1:E:255:ASP:O	1:E:258:GLU:HB3	2.09	0.51
1:E:190:ALA:HB1	1:E:197:VAL:HG13	1.93	0.51
1:F:134:GLU:HB3	1:F:196:ARG:HG3	1.93	0.51
1:D:104:HIS:HE2	4:D:381:CIT:H21	1.76	0.51
1:E:208:GLY:HA2	1:E:284:TRP:CE2	2.46	0.51
1:F:240:ARG:HH11	1:F:244:ASN:HD21	1.59	0.51
1:C:309:LYS:NZ	1:D:167:ARG:CD	2.71	0.50
1:A:261:ARG:HG2	1:A:265:GLN:HE21	1.76	0.50
1:D:153:PHE:HD1	1:D:158:GLN:HG3	1.76	0.50
1:A:371:ASP:OD1	1:H:269:TRP:HB2	2.11	0.50
1:G:344:ARG:CG	1:G:349:GLU:HB2	2.35	0.50
1:C:240:ARG:NH1	1:C:244:ASN:HD22	2.08	0.50
1:E:299:ILE:HD11	1:E:323:ILE:HB	1.92	0.50
1:C:153:PHE:HD1	1:C:158:GLN:HG3	1.74	0.50
1:A:153:PHE:HD1	1:A:158:GLN:HG3	1.76	0.50
1:H:153:PHE:HD1	1:H:158:GLN:HG3	1.76	0.50
1:B:80:PRO:HB2	1:B:362:TRP:CZ3	2.47	0.50
1:H:152:ILE:HG21	1:H:204:LEU:HD12	1.94	0.50
1:H:357:GLU:O	1:H:361:ARG:HD3	2.11	0.50
1:A:190:ALA:HB1	1:A:197:VAL:HG13	1.93	0.50
1:G:114:HIS:O	1:G:117:SER:HB3	2.11	0.50
1:H:140:ARG:HD3	1:H:370:LEU:HD21	1.93	0.50
1:H:370:LEU:N	1:H:370:LEU:HD12	2.26	0.50
1:B:223:LEU:HD23	1:C:223:LEU:HD23	1.93	0.50
1:D:258:GLU:OE1	1:D:261:ARG:HB3	2.11	0.50
1:F:260:VAL:HG13	1:F:311:PHE:CE1	2.46	0.50
1:G:328:VAL:O	1:G:330:PRO:HD3	2.11	0.50
1:F:357:GLU:HG2	1:F:361:ARG:HH21	1.76	0.50
1:B:153:PHE:CD1	1:B:158:GLN:HG3	2.46	0.50
1:B:369:TYR:CD1	1:B:370:LEU:N	2.80	0.50
1:H:72:VAL:HG21	1:H:342:ALA:CB	2.37	0.50
1:A:152:ILE:HG21	1:A:204:LEU:HD12	1.94	0.50
1:E:81:ILE:O	1:E:132:VAL:HA	2.10	0.50
1:D:114:HIS:O	1:D:117:SER:HB3	2.12	0.50
1:H:245:GLY:HA2	1:H:249:ALA:HB2	1.93	0.50
1:E:5:LEU:HB2	1:E:68:PHE:CE2	2.47	0.50
1:G:299:ILE:HD11	1:G:323:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:LYS:HD3	1:G:29:ASN:HD22	1.76	0.49
1:F:53:ILE:O	1:F:56:GLN:HB3	2.12	0.49
1:E:70:ALA:HA	1:E:122:VAL:HG12	1.93	0.49
1:H:5:LEU:HB2	1:H:68:PHE:CE2	2.46	0.49
1:E:255:ASP:OD1	1:E:258:GLU:N	2.44	0.49
1:G:245:GLY:O	1:G:248:VAL:HG12	2.12	0.49
1:F:306:ALA:HB3	1:F:330:PRO:HA	1.93	0.49
1:E:214:ARG:HG2	1:E:242:VAL:HA	1.94	0.49
1:C:238:LYS:O	1:C:242:VAL:HG22	2.11	0.49
1:F:299:ILE:HD11	1:F:323:ILE:HB	1.94	0.49
1:D:299:ILE:HD11	1:D:323:ILE:HB	1.94	0.49
1:F:208:GLY:HA2	1:F:284:TRP:CZ2	2.48	0.49
1:C:251:LEU:HD21	1:C:270:ALA:HA	1.94	0.49
1:F:238:LYS:HZ3	1:F:238:LYS:HB2	1.77	0.49
1:F:81:ILE:O	1:F:132:VAL:HA	2.12	0.49
1:D:152:ILE:HG21	1:D:204:LEU:HD12	1.93	0.49
1:E:240:ARG:HA	1:E:244:ASN:HD21	1.77	0.49
1:E:153:PHE:HD1	1:E:158:GLN:HG3	1.76	0.49
1:C:208:GLY:HA2	1:C:284:TRP:CZ2	2.46	0.49
1:F:314:PRO:O	1:F:318:LYS:HG3	2.13	0.49
1:B:153:PHE:HD1	1:B:158:GLN:HG3	1.77	0.49
1:A:344:ARG:CG	1:A:349:GLU:HB2	2.36	0.49
1:A:240:ARG:NH1	1:A:244:ASN:OD1	2.46	0.49
1:E:187:ILE:HG13	1:E:211:THR:HG22	1.95	0.49
1:G:51:GLU:OE2	1:G:55:ARG:NH1	2.43	0.49
1:D:245:GLY:HA2	1:D:249:ALA:HB2	1.95	0.49
1:B:93:ILE:N	1:B:93:ILE:HD12	2.26	0.49
1:E:57:PHE:O	1:E:61:THR:HG23	2.12	0.49
1:E:242:VAL:O	1:E:242:VAL:HG13	2.12	0.49
1:C:93:ILE:HD13	1:C:114:HIS:CD2	2.48	0.49
1:C:299:ILE:HD11	1:C:323:ILE:HB	1.94	0.49
1:C:15:LYS:HD3	1:C:29:ASN:HD22	1.78	0.49
1:C:307:HIS:HA	1:C:309:LYS:HE3	1.95	0.49
1:G:209:PRO:HB3	1:G:280:GLN:HB3	1.95	0.49
1:G:306:ALA:HB3	1:G:330:PRO:HA	1.95	0.49
1:H:43:ILE:C	1:H:45:ASP:N	2.64	0.49
1:B:204:LEU:O	1:B:242:VAL:HG22	2.13	0.49
1:D:82:PRO:HD2	1:D:358:GLU:CG	2.41	0.48
1:E:209:PRO:HB3	1:E:280:GLN:HB3	1.95	0.48
1:E:251:LEU:CD2	1:E:270:ALA:HA	2.43	0.48
1:B:244:ASN:CG	1:B:245:GLY:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ARG:HH22	1:C:365:ARG:NH1	2.01	0.48
1:B:220:LEU:HD22	1:C:223:LEU:HD22	1.94	0.48
1:G:152:ILE:HG21	1:G:204:LEU:HD12	1.94	0.48
1:F:241:ILE:HG23	1:G:220:LEU:HD12	1.94	0.48
1:H:333:ASN:ND2	1:H:336:LYS:HB2	2.27	0.48
1:G:23:ARG:HG3	1:G:23:ARG:NH1	2.28	0.48
1:C:72:VAL:HG21	1:C:342:ALA:CB	2.42	0.48
1:H:117:SER:HB2	1:H:124:ALA:HB2	1.96	0.48
1:H:59:GLU:O	1:H:61:THR:N	2.46	0.48
1:A:154:HIS:HB3	6:A:401:HOH:O	2.13	0.48
1:A:92:MET:HG2	1:A:92:MET:O	2.12	0.48
1:A:15:LYS:HD3	1:A:29:ASN:HD22	1.77	0.48
1:E:152:ILE:HG21	1:E:204:LEU:HD12	1.95	0.48
1:B:3:ARG:NE	1:B:63:TYR:CE2	2.82	0.48
1:B:147:TYR:CD1	1:B:147:TYR:N	2.81	0.48
1:H:314:PRO:O	1:H:318:LYS:HG3	2.13	0.48
1:H:299:ILE:HD11	1:H:323:ILE:HB	1.95	0.48
1:H:133:ASP:OD1	1:H:140:ARG:NH2	2.46	0.48
1:G:314:PRO:O	1:G:318:LYS:HG3	2.13	0.48
1:C:79:ASP:O	1:C:81:ILE:HG23	2.13	0.48
1:G:147:TYR:N	1:G:147:TYR:CD1	2.82	0.48
1:A:117:SER:HB2	1:A:124:ALA:HB2	1.96	0.48
1:C:311:PHE:O	1:C:314:PRO:HD2	2.14	0.48
1:F:360:ARG:O	1:F:364:GLU:HB2	2.13	0.48
1:C:209:PRO:HD3	1:C:284:TRP:CD2	2.49	0.48
1:G:55:ARG:NH2	1:G:119:GLU:OE1	2.46	0.48
1:F:362:TRP:C	1:F:364:GLU:H	2.16	0.48
1:B:258:GLU:OE1	1:B:261:ARG:HD2	2.14	0.48
1:A:370:LEU:O	1:A:373:ILE:HG12	2.13	0.48
1:E:333:ASN:C	1:E:333:ASN:HD22	2.15	0.48
1:A:23:ARG:HH21	1:B:307:HIS:CD2	2.31	0.48
1:H:23:ARG:N	1:H:23:ARG:HD2	2.29	0.48
1:F:238:LYS:HE3	1:G:221:THR:HG23	1.96	0.48
1:E:117:SER:HB2	1:E:124:ALA:HB2	1.96	0.48
1:A:299:ILE:HD11	1:A:323:ILE:HB	1.95	0.48
1:H:128:ASP:HB2	1:H:156:LEU:HA	1.95	0.48
1:A:55:ARG:HH22	1:A:119:GLU:CD	2.16	0.48
1:E:72:VAL:HG21	1:E:342:ALA:CB	2.42	0.48
1:G:74:ARG:NH2	1:G:156:LEU:HB3	2.29	0.48
1:F:357:GLU:HG2	1:F:361:ARG:NH2	2.29	0.48
1:B:117:SER:HB2	1:B:124:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ARG:HG2	1:G:265:GLN:HE21	1.78	0.47
1:D:40:PHE:CD1	1:D:40:PHE:N	2.81	0.47
1:B:152:ILE:HG21	1:B:204:LEU:HD12	1.95	0.47
1:B:209:PRO:HB3	1:B:280:GLN:HB3	1.96	0.47
1:A:147:TYR:CD1	1:A:147:TYR:N	2.82	0.47
1:B:223:LEU:HD21	1:C:224:VAL:CG2	2.44	0.47
1:H:209:PRO:HB3	1:H:280:GLN:HB3	1.96	0.47
1:A:314:PRO:O	1:A:318:LYS:HG3	2.13	0.47
1:B:299:ILE:HD11	1:B:323:ILE:HB	1.97	0.47
1:B:1:MET:HA	1:B:21:ASP:OD2	2.13	0.47
1:E:22:GLU:OE2	1:E:347:ARG:NH2	2.47	0.47
1:A:240:ARG:HD2	1:A:244:ASN:HB3	1.97	0.47
1:E:314:PRO:O	1:E:318:LYS:HG3	2.14	0.47
1:D:209:PRO:HB3	1:D:280:GLN:HB3	1.97	0.47
1:A:224:VAL:HG21	1:H:241:ILE:HD11	1.96	0.47
1:F:364:GLU:O	1:F:368:SER:N	2.47	0.47
1:A:332:SER:O	1:A:334:GLU:HG3	2.14	0.47
1:A:183:MET:HB3	1:A:305:LEU:HD12	1.95	0.47
1:B:15:LYS:HD3	1:B:29:ASN:HD22	1.79	0.47
1:B:255:ASP:O	1:B:259:VAL:HG23	2.13	0.47
1:H:242:VAL:HG13	1:H:242:VAL:O	2.15	0.47
1:E:258:GLU:O	1:E:261:ARG:HB3	2.13	0.47
1:H:78:LEU:CD2	1:H:92:MET:HG3	2.44	0.47
1:E:26:LYS:HE3	1:F:28:GLN:OE1	2.15	0.47
1:E:165:VAL:HG22	1:E:329:PHE:HE2	1.79	0.47
1:B:260:VAL:HG13	1:B:311:PHE:CE1	2.49	0.47
1:B:314:PRO:O	1:B:318:LYS:HG3	2.15	0.47
1:F:209:PRO:HB3	1:F:280:GLN:HB3	1.96	0.47
1:C:209:PRO:HB3	1:C:280:GLN:HB3	1.97	0.47
1:B:159:LYS:O	1:B:163:LYS:HG3	2.15	0.47
1:C:147:TYR:N	1:C:147:TYR:CD1	2.82	0.47
1:E:147:TYR:CD1	1:E:147:TYR:N	2.82	0.47
1:E:244:ASN:O	1:E:249:ALA:HB2	2.14	0.47
1:H:238:LYS:HB2	1:H:238:LYS:HZ2	1.78	0.47
1:F:93:ILE:HD13	1:F:114:HIS:CD2	2.50	0.47
1:A:209:PRO:HB3	1:A:280:GLN:HB3	1.96	0.47
1:D:135:MET:HA	1:D:198:ILE:HA	1.97	0.47
1:D:247:LEU:HD23	1:D:273:VAL:HG12	1.97	0.47
1:F:117:SER:HB2	1:F:124:ALA:HB2	1.95	0.47
1:D:39:ARG:HB3	1:D:40:PHE:CD1	2.49	0.47
1:A:305:LEU:HB3	1:A:312:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:LEU:O	1:F:242:VAL:HG22	2.15	0.47
1:C:240:ARG:HH11	1:C:244:ASN:HD22	1.63	0.47
1:C:117:SER:HB2	1:C:124:ALA:HB2	1.96	0.47
1:F:15:LYS:HD3	1:F:29:ASN:HD22	1.80	0.47
1:F:144:HIS:CE1	1:G:240:ARG:HH21	2.33	0.47
1:H:147:TYR:N	1:H:147:TYR:CD1	2.82	0.47
1:D:147:TYR:CD1	1:D:147:TYR:N	2.83	0.47
1:E:169:MET:O	1:E:171:LYS:HG3	2.15	0.47
1:A:54:ALA:O	1:A:57:PHE:HB3	2.15	0.47
1:A:307:HIS:HA	1:A:309:LYS:HE3	1.97	0.47
1:B:88:VAL:HG12	1:B:93:ILE:CD1	2.36	0.46
1:A:242:VAL:O	1:A:242:VAL:HG12	2.15	0.46
1:D:130:VAL:O	1:D:152:ILE:HA	2.15	0.46
1:G:204:LEU:O	1:G:242:VAL:HG21	2.15	0.46
1:C:240:ARG:NH1	1:C:244:ASN:ND2	2.63	0.46
1:D:134:GLU:HB2	1:D:196:ARG:NH1	2.30	0.46
1:B:272:ARG:HD2	1:C:369:TYR:CD1	2.50	0.46
1:H:305:LEU:HB3	1:H:312:LEU:CD2	2.45	0.46
1:C:187:ILE:HG13	1:C:211:THR:HG22	1.97	0.46
1:H:72:VAL:HG12	1:H:338:LEU:HD22	1.96	0.46
1:A:208:GLY:HA2	1:A:284:TRP:CZ2	2.49	0.46
1:G:305:LEU:HB3	1:G:312:LEU:CD2	2.46	0.46
1:D:117:SER:HB2	1:D:124:ALA:HB2	1.96	0.46
1:G:117:SER:HB2	1:G:124:ALA:HB2	1.97	0.46
1:H:307:HIS:HA	1:H:309:LYS:HE3	1.97	0.46
1:E:362:TRP:O	1:E:365:ARG:HB3	2.15	0.46
1:E:311:PHE:O	1:E:314:PRO:HD2	2.16	0.46
1:A:233:THR:OG1	1:A:236:GLU:HB3	2.16	0.46
1:C:71:PHE:HE1	1:C:122:VAL:HB	1.81	0.46
1:B:219:PRO:HG2	1:B:222:GLN:NE2	2.29	0.46
1:F:372:GLY:HA3	1:G:269:TRP:CE3	2.50	0.46
1:G:253:THR:HG21	1:G:259:VAL:HG22	1.97	0.46
1:F:56:GLN:O	1:F:60:GLU:HG2	2.15	0.46
1:C:208:GLY:HA2	1:C:284:TRP:CE2	2.51	0.46
1:A:79:ASP:O	1:A:81:ILE:HG23	2.15	0.46
1:H:15:LYS:HD3	1:H:29:ASN:HD22	1.81	0.46
1:G:104:HIS:H	1:G:107:ASN:HD22	1.64	0.46
1:D:258:GLU:OE1	1:D:261:ARG:HD2	2.15	0.46
1:H:79:ASP:HB2	1:H:363:ARG:HH12	1.80	0.46
1:C:128:ASP:HB2	1:C:156:LEU:HA	1.97	0.46
1:D:165:VAL:HG21	1:D:300:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:HG13	1:A:311:PHE:CE1	2.50	0.46
1:D:169:MET:O	1:D:171:LYS:HG3	2.15	0.46
1:D:208:GLY:HA2	1:D:284:TRP:CE2	2.50	0.46
1:C:314:PRO:O	1:C:318:LYS:HG3	2.15	0.46
1:C:251:LEU:CD2	1:C:270:ALA:HA	2.46	0.46
1:B:233:THR:OG1	1:B:236:GLU:HB3	2.16	0.46
1:F:305:LEU:HB3	1:F:312:LEU:CD2	2.46	0.46
1:G:200:VAL:HG22	1:G:201:ASN:N	2.31	0.46
1:E:306:ALA:CB	1:E:330:PRO:HA	2.42	0.46
1:F:208:GLY:HA2	1:F:284:TRP:CE2	2.50	0.46
1:G:307:HIS:HA	1:G:309:LYS:HE3	1.98	0.46
1:D:327:LEU:HB3	1:D:329:PHE:HE1	1.80	0.46
1:D:233:THR:OG1	1:D:236:GLU:HB3	2.16	0.46
1:C:61:THR:HG22	1:C:61:THR:O	2.16	0.46
1:D:88:VAL:HG12	1:D:93:ILE:CD1	2.34	0.46
1:E:144:HIS:HE1	1:E:146:ASN:ND2	2.13	0.46
1:F:257:ARG:HB3	1:F:257:ARG:HH11	1.81	0.46
1:A:306:ALA:HB3	1:A:330:PRO:HA	1.98	0.46
1:C:159:LYS:O	1:C:163:LYS:HG3	2.15	0.46
1:F:200:VAL:HG22	1:F:201:ASN:N	2.31	0.46
1:E:39:ARG:O	1:E:39:ARG:HG2	2.15	0.46
1:E:305:LEU:HB3	1:E:312:LEU:CD2	2.46	0.45
1:B:247:LEU:HD23	1:B:273:VAL:HG12	1.99	0.45
1:C:333:ASN:ND2	1:C:336:LYS:CB	2.72	0.45
1:D:104:HIS:HD2	1:D:204:LEU:HD21	1.81	0.45
1:E:165:VAL:HG21	1:E:300:VAL:HG21	1.98	0.45
1:D:200:VAL:HG22	1:D:201:ASN:N	2.31	0.45
1:B:16:LEU:HD11	1:B:54:ALA:HA	1.98	0.45
1:D:136:GLU:HB3	1:D:138:VAL:HG12	1.97	0.45
1:D:159:LYS:O	1:D:163:LYS:HG3	2.16	0.45
1:G:257:ARG:HG2	1:G:257:ARG:NH1	2.31	0.45
1:E:165:VAL:HG22	1:E:329:PHE:CE2	2.52	0.45
1:E:183:MET:HB3	1:E:305:LEU:HD12	1.97	0.45
1:B:183:MET:HB3	1:B:305:LEU:HD12	1.98	0.45
1:C:305:LEU:HB3	1:C:312:LEU:CD2	2.46	0.45
1:F:48:GLU:O	1:F:52:LYS:HG3	2.16	0.45
1:C:1:MET:HA	1:C:21:ASP:OD2	2.17	0.45
1:C:130:VAL:O	1:C:130:VAL:HG22	2.16	0.45
1:B:305:LEU:HB3	1:B:312:LEU:CD2	2.47	0.45
1:E:233:THR:OG1	1:E:236:GLU:HB3	2.15	0.45
1:D:361:ARG:O	1:D:365:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:ASP:O	1:H:81:ILE:HG23	2.16	0.45
1:D:224:VAL:HG21	1:E:241:ILE:HD11	1.97	0.45
1:D:70:ALA:HA	1:D:122:VAL:CG1	2.47	0.45
1:B:289:ALA:HB2	1:B:323:ILE:HD13	1.99	0.45
1:C:183:MET:HB3	1:C:305:LEU:HD12	1.97	0.45
1:A:227:CYS:HG	1:H:227:CYS:HG	1.64	0.45
1:F:82:PRO:HD2	1:F:358:GLU:HG3	1.99	0.45
1:D:305:LEU:HB3	1:D:312:LEU:CD2	2.46	0.45
1:C:233:THR:OG1	1:C:236:GLU:HB3	2.16	0.45
1:C:239:LYS:HG2	1:C:244:ASN:OD1	2.15	0.45
1:H:157:ASN:HD21	1:H:161:VAL:HG13	1.80	0.45
1:F:289:ALA:HB2	1:F:323:ILE:HD13	1.99	0.45
1:F:79:ASP:O	1:F:81:ILE:HG23	2.17	0.45
1:D:55:ARG:NH2	1:D:119:GLU:OE1	2.49	0.45
1:A:159:LYS:O	1:A:163:LYS:HG3	2.16	0.45
1:H:233:THR:OG1	1:H:236:GLU:HB3	2.17	0.45
1:D:15:LYS:HD3	1:D:29:ASN:HD22	1.81	0.45
1:B:200:VAL:HG22	1:B:201:ASN:N	2.32	0.45
1:B:257:ARG:NH2	1:B:257:ARG:HB3	2.31	0.45
1:E:370:LEU:HD12	1:E:370:LEU:N	2.31	0.45
1:D:8:ASN:ND2	1:D:334:GLU:HB3	2.31	0.45
1:C:361:ARG:O	1:C:364:GLU:HB2	2.17	0.45
1:A:200:VAL:HG22	1:A:201:ASN:N	2.32	0.45
1:E:15:LYS:HD3	1:E:29:ASN:HD22	1.82	0.45
1:H:80:PRO:HB2	1:H:362:TRP:CE3	2.51	0.45
1:B:258:GLU:O	1:B:261:ARG:HB3	2.17	0.45
1:E:247:LEU:HD23	1:E:273:VAL:HG12	1.98	0.45
1:E:159:LYS:O	1:E:163:LYS:HG3	2.17	0.45
1:F:260:VAL:O	1:F:264:LYS:HG3	2.17	0.45
1:D:307:HIS:HA	1:D:309:LYS:HE3	1.99	0.45
1:D:370:LEU:HD11	1:E:269:TRP:HZ3	1.81	0.45
1:H:88:VAL:HG23	1:H:124:ALA:O	2.17	0.44
1:H:104:HIS:ND1	1:H:105:ALA:N	2.65	0.44
1:H:183:MET:HB3	1:H:305:LEU:HD12	1.99	0.44
1:F:183:MET:HB3	1:F:305:LEU:HD12	1.99	0.44
1:G:144:HIS:CE1	1:G:146:ASN:HD22	2.35	0.44
1:E:357:GLU:O	1:E:361:ARG:HG2	2.17	0.44
1:D:93:ILE:HD13	1:D:114:HIS:CG	2.52	0.44
1:B:79:ASP:O	1:B:81:ILE:HG23	2.17	0.44
1:A:70:ALA:HA	1:A:122:VAL:CG1	2.47	0.44
1:G:71:PHE:HE1	1:G:122:VAL:HB	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:THR:OG1	1:F:236:GLU:HB3	2.17	0.44
1:G:233:THR:OG1	1:G:236:GLU:HB3	2.16	0.44
1:H:208:GLY:HA2	1:H:284:TRP:CE2	2.51	0.44
1:E:200:VAL:HG22	1:E:201:ASN:N	2.32	0.44
1:B:40:PHE:CD1	1:B:40:PHE:N	2.85	0.44
1:B:104:HIS:CD2	1:B:105:ALA:N	2.85	0.44
1:F:70:ALA:HA	1:F:122:VAL:CG1	2.48	0.44
1:G:159:LYS:O	1:G:163:LYS:HG3	2.17	0.44
1:B:344:ARG:CG	1:B:349:GLU:HB2	2.48	0.44
1:A:88:VAL:HG23	1:A:124:ALA:O	2.18	0.44
1:G:364:GLU:O	1:G:367:ASP:N	2.49	0.44
1:E:240:ARG:HD2	1:E:244:ASN:CG	2.37	0.44
1:G:251:LEU:HD21	1:G:270:ALA:HA	1.99	0.44
1:E:71:PHE:HE1	1:E:122:VAL:HB	1.83	0.44
1:G:219:PRO:HG2	1:G:222:GLN:NE2	2.32	0.44
1:A:369:TYR:CD1	1:H:272:ARG:NH2	2.86	0.44
1:D:344:ARG:CG	1:D:349:GLU:HB2	2.38	0.44
1:F:81:ILE:HG22	1:F:359:SER:HA	2.00	0.44
1:E:333:ASN:ND2	1:E:336:LYS:H	2.15	0.44
1:G:16:LEU:HD11	1:G:54:ALA:HA	1.98	0.44
1:E:17:SER:HG	1:E:19:PHE:HE1	1.65	0.44
1:H:165:VAL:HG21	1:H:300:VAL:HG21	2.00	0.44
1:G:311:PHE:O	1:G:314:PRO:HD2	2.18	0.44
1:B:70:ALA:HA	1:B:122:VAL:CG1	2.47	0.44
1:H:43:ILE:HD12	1:H:104:HIS:N	2.32	0.44
1:A:361:ARG:O	1:A:365:ARG:HG3	2.18	0.44
1:A:370:LEU:C	1:A:372:GLY:H	2.21	0.44
1:G:1:MET:HA	1:G:21:ASP:OD2	2.18	0.44
1:A:1:MET:HA	1:A:21:ASP:OD2	2.17	0.44
1:C:260:VAL:O	1:C:264:LYS:HG3	2.18	0.44
1:D:104:HIS:H	1:D:107:ASN:HD22	1.64	0.44
1:B:165:VAL:HG21	1:B:300:VAL:HG21	2.00	0.44
1:B:318:LYS:HB2	6:B:408:HOH:O	2.18	0.44
1:E:79:ASP:O	1:E:81:ILE:HG23	2.17	0.44
1:A:55:ARG:NH2	1:A:119:GLU:OE2	2.51	0.44
1:A:272:ARG:NH2	1:H:370:LEU:HG	2.32	0.44
1:F:165:VAL:HG21	1:F:300:VAL:HG21	1.99	0.43
1:F:165:VAL:HG22	1:F:329:PHE:CZ	2.53	0.43
1:B:157:ASN:HD21	1:B:161:VAL:HG13	1.82	0.43
1:A:238:LYS:HB2	1:A:238:LYS:HZ3	1.82	0.43
1:G:70:ALA:HA	1:G:122:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HB2	1:A:373:ILE:HG23	2.00	0.43
1:C:200:VAL:HG22	1:C:201:ASN:N	2.32	0.43
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.83	0.43
1:G:93:ILE:HD13	1:G:114:HIS:CG	2.53	0.43
1:D:104:HIS:H	1:D:107:ASN:ND2	2.15	0.43
1:D:241:ILE:HD12	1:E:224:VAL:HG21	1.99	0.43
1:B:311:PHE:O	1:B:314:PRO:HD2	2.18	0.43
1:E:251:LEU:HD12	1:E:259:VAL:HG22	1.99	0.43
1:C:311:PHE:C	1:C:314:PRO:HD2	2.39	0.43
1:B:248:VAL:O	1:B:252:GLY:N	2.50	0.43
1:C:153:PHE:CE1	1:C:155:ALA:HA	2.53	0.43
1:C:177:ASN:HA	1:C:192:HIS:O	2.19	0.43
1:G:366:TYR:O	1:G:370:LEU:HG	2.17	0.43
1:D:144:HIS:CE1	1:D:146:ASN:HD22	2.36	0.43
1:C:165:VAL:HG21	1:C:300:VAL:HG21	1.99	0.43
1:B:213:GLU:HA	1:B:245:GLY:O	2.18	0.43
1:F:357:GLU:O	1:F:361:ARG:HG2	2.19	0.43
1:H:289:ALA:HB2	1:H:323:ILE:HD13	2.00	0.43
1:G:183:MET:HB3	1:G:305:LEU:HD12	2.00	0.43
1:G:169:MET:O	1:G:171:LYS:HG3	2.18	0.43
1:G:167:ARG:CD	1:H:309:LYS:NZ	2.75	0.43
1:G:255:ASP:HB3	1:G:258:GLU:HB2	1.99	0.43
1:G:165:VAL:HG21	1:G:300:VAL:HG21	2.00	0.43
1:H:70:ALA:HA	1:H:122:VAL:CG1	2.48	0.43
1:B:209:PRO:HD3	1:B:284:TRP:CD2	2.53	0.43
1:G:104:HIS:H	1:G:107:ASN:ND2	2.16	0.43
1:G:88:VAL:HG23	1:G:124:ALA:O	2.19	0.43
1:B:283:LYS:HB3	1:C:287:LYS:HG3	2.01	0.43
1:H:366:TYR:HA	1:H:370:LEU:HD13	2.00	0.43
1:A:71:PHE:HE1	1:A:122:VAL:HB	1.83	0.43
1:C:55:ARG:NH2	1:C:119:GLU:OE2	2.50	0.43
1:F:250:TYR:HB3	1:F:273:VAL:HG21	2.00	0.43
1:F:275:ARG:HH12	1:G:138:VAL:HB	1.83	0.43
1:D:88:VAL:HG23	1:D:124:ALA:O	2.19	0.43
1:H:137:ASP:HA	1:H:140:ARG:HG3	2.01	0.43
1:B:26:LYS:CD	1:B:61:THR:HG22	2.48	0.43
1:F:157:ASN:HD21	1:F:161:VAL:HG13	1.82	0.43
1:D:183:MET:HB3	1:D:305:LEU:HD12	1.99	0.43
1:C:55:ARG:HH22	1:C:119:GLU:CD	2.21	0.43
1:A:246:GLY:O	1:A:250:TYR:HD1	2.02	0.43
1:H:159:LYS:O	1:H:163:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:GLU:OE1	1:F:268:GLU:HA	2.19	0.43
1:B:88:VAL:HG23	1:B:124:ALA:O	2.18	0.43
1:E:255:ASP:OD2	1:E:257:ARG:NH1	2.51	0.43
1:A:165:VAL:HG21	1:A:300:VAL:HG21	2.00	0.43
1:G:209:PRO:HA	1:G:280:GLN:OE1	2.19	0.43
1:F:307:HIS:HA	1:F:309:LYS:HE3	2.00	0.43
1:C:23:ARG:HH11	1:C:23:ARG:HG3	1.83	0.43
1:B:268:GLU:HA	1:B:268:GLU:OE1	2.19	0.43
1:B:280:GLN:O	1:B:284:TRP:HE3	2.01	0.43
1:F:159:LYS:O	1:F:163:LYS:HG3	2.19	0.43
1:D:16:LEU:HD11	1:D:54:ALA:HA	2.00	0.43
1:F:104:HIS:H	1:F:107:ASN:HD22	1.66	0.43
1:C:16:LEU:HD11	1:C:54:ALA:HA	2.01	0.43
1:C:157:ASN:HD21	1:C:161:VAL:HG13	1.84	0.43
1:B:260:VAL:O	1:B:264:LYS:HG3	2.19	0.43
1:A:311:PHE:O	1:A:314:PRO:HD2	2.19	0.43
1:B:245:GLY:O	1:B:248:VAL:HG12	2.18	0.43
1:F:255:ASP:O	1:F:258:GLU:HB3	2.19	0.43
1:A:153:PHE:CE1	1:A:155:ALA:HA	2.54	0.43
1:F:144:HIS:CE1	1:F:146:ASN:HD22	2.37	0.43
1:D:8:ASN:HD21	1:D:334:GLU:HB3	1.83	0.43
1:B:287:LYS:HG3	1:C:283:LYS:HB3	2.01	0.43
1:H:80:PRO:HB2	1:H:362:TRP:CZ3	2.54	0.43
1:D:311:PHE:O	1:D:314:PRO:HD2	2.18	0.43
1:A:208:GLY:HA2	1:A:284:TRP:CE2	2.53	0.43
1:E:20:GLU:O	1:E:21:ASP:HB2	2.18	0.43
1:H:200:VAL:HG22	1:H:201:ASN:N	2.33	0.43
1:G:315:TRP:O	1:G:319:ARG:HG3	2.19	0.43
1:D:78:LEU:CD2	1:D:92:MET:HG3	2.49	0.42
1:H:16:LEU:HD11	1:H:54:ALA:HA	2.01	0.42
1:E:351:LYS:HA	1:E:352:PRO:HD3	1.93	0.42
1:F:209:PRO:HD3	1:F:284:TRP:CD2	2.54	0.42
1:C:289:ALA:HB2	1:C:323:ILE:HD13	2.00	0.42
1:H:333:ASN:HD22	1:H:336:LYS:CB	2.32	0.42
1:B:208:GLY:HA2	1:B:284:TRP:CE2	2.53	0.42
1:D:363:ARG:C	1:D:365:ARG:H	2.23	0.42
1:E:177:ASN:HA	1:E:192:HIS:O	2.19	0.42
1:A:177:ASN:HA	1:A:192:HIS:O	2.19	0.42
1:H:1:MET:HA	1:H:21:ASP:OD2	2.19	0.42
1:D:268:GLU:OE1	1:D:268:GLU:HA	2.19	0.42
1:A:157:ASN:HD21	1:A:161:VAL:HG13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LYS:HB2	1:C:238:LYS:HZ2	1.83	0.42
1:F:100:LYS:HG3	1:F:101:ASN:N	2.34	0.42
1:B:244:ASN:CG	1:B:245:GLY:H	2.23	0.42
1:F:71:PHE:HE1	1:F:122:VAL:HB	1.84	0.42
1:F:209:PRO:HA	1:F:280:GLN:OE1	2.20	0.42
1:A:80:PRO:HB2	1:A:362:TRP:CZ3	2.54	0.42
1:D:93:ILE:O	1:D:93:ILE:CG2	2.67	0.42
1:D:223:LEU:HD21	1:E:224:VAL:HG23	2.01	0.42
1:B:144:HIS:CE1	1:B:146:ASN:HD22	2.37	0.42
1:A:100:LYS:HG3	1:A:101:ASN:N	2.35	0.42
1:E:311:PHE:C	1:E:314:PRO:HD2	2.39	0.42
1:C:70:ALA:HA	1:C:122:VAL:CG1	2.49	0.42
1:A:78:LEU:CD2	1:A:92:MET:HG3	2.49	0.42
1:D:74:ARG:NH1	1:D:130:VAL:HG12	2.35	0.42
1:E:209:PRO:HA	1:E:280:GLN:OE1	2.19	0.42
1:D:100:LYS:HG3	1:D:101:ASN:N	2.35	0.42
1:F:78:LEU:CD2	1:F:92:MET:HG3	2.49	0.42
1:F:88:VAL:HG12	1:F:93:ILE:HD11	2.02	0.42
1:F:18:ILE:HG13	1:F:57:PHE:CE2	2.55	0.42
1:C:209:PRO:HA	1:C:280:GLN:OE1	2.19	0.42
1:H:345:VAL:CG1	1:H:352:PRO:HG3	2.49	0.42
1:A:268:GLU:HA	1:A:268:GLU:OE1	2.19	0.42
1:A:22:GLU:OE1	1:A:22:GLU:N	2.49	0.42
1:H:92:MET:CG	1:H:92:MET:O	2.64	0.42
1:D:223:LEU:HD21	1:E:224:VAL:HG22	2.00	0.42
1:C:241:ILE:HG13	1:C:242:VAL:N	2.35	0.42
1:D:248:VAL:HG22	1:D:254:SER:HB2	2.02	0.42
1:E:28:GLN:OE1	1:F:26:LYS:HE3	2.20	0.42
1:E:289:ALA:HB2	1:E:323:ILE:HD13	2.02	0.42
1:B:369:TYR:O	1:C:269:TRP:CZ3	2.73	0.42
1:F:1:MET:HA	1:F:21:ASP:OD2	2.20	0.42
1:E:268:GLU:HA	1:E:268:GLU:OE1	2.19	0.42
1:H:260:VAL:O	1:H:264:LYS:HG3	2.20	0.42
1:B:307:HIS:HA	1:B:309:LYS:HE3	2.00	0.42
1:D:209:PRO:HA	1:D:280:GLN:OE1	2.20	0.42
1:G:257:ARG:HH11	1:G:257:ARG:HG2	1.85	0.42
1:F:104:HIS:ND1	1:F:105:ALA:N	2.68	0.42
1:B:169:MET:O	1:B:171:LYS:HG3	2.20	0.42
1:D:144:HIS:CE1	1:E:240:ARG:HH21	2.38	0.42
1:B:306:ALA:CB	1:B:330:PRO:HA	2.48	0.42
1:H:153:PHE:CE1	1:H:155:ALA:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TYR:C	1:A:369:TYR:CD1	2.93	0.42
1:D:127:VAL:O	1:D:128:ASP:C	2.58	0.42
1:D:248:VAL:CG2	1:D:254:SER:HB2	2.49	0.42
1:F:153:PHE:CE1	1:F:155:ALA:HA	2.55	0.42
1:D:138:VAL:HB	1:E:275:ARG:HH12	1.83	0.42
1:H:8:ASN:ND2	1:H:334:GLU:OE2	2.52	0.42
1:B:345:VAL:CG1	1:B:352:PRO:HG3	2.50	0.42
1:B:72:VAL:HG12	1:B:338:LEU:HD22	2.01	0.42
1:A:283:LYS:HB3	1:H:287:LYS:HG3	2.01	0.42
1:D:1:MET:HA	1:D:21:ASP:OD2	2.20	0.42
1:F:96:LEU:CD1	1:F:110:ALA:HB3	2.50	0.42
1:G:78:LEU:HD21	1:G:92:MET:HG3	2.01	0.42
1:H:96:LEU:CD1	1:H:110:ALA:HB3	2.50	0.42
1:F:335:GLU:OE2	1:F:335:GLU:N	2.50	0.42
1:E:344:ARG:CG	1:E:349:GLU:HB2	2.36	0.41
1:H:250:TYR:HB2	1:H:273:VAL:HG11	2.02	0.41
1:D:311:PHE:C	1:D:314:PRO:HD2	2.41	0.41
1:B:199:ASP:OD1	1:B:200:VAL:N	2.53	0.41
1:H:22:GLU:OE2	1:H:347:ARG:NH2	2.51	0.41
1:C:367:ASP:O	1:C:368:SER:C	2.59	0.41
1:H:144:HIS:CE1	1:H:146:ASN:HD22	2.38	0.41
1:G:100:LYS:HG3	1:G:101:ASN:N	2.35	0.41
1:B:311:PHE:C	1:B:314:PRO:HD2	2.40	0.41
1:E:100:LYS:HG3	1:E:101:ASN:N	2.35	0.41
1:F:136:GLU:OE1	1:F:193:ARG:NH2	2.53	0.41
1:H:177:ASN:HA	1:H:192:HIS:O	2.20	0.41
1:D:250:TYR:O	1:D:251:LEU:HD23	2.20	0.41
1:E:16:LEU:HD11	1:E:54:ALA:HA	2.02	0.41
1:H:209:PRO:HA	1:H:280:GLN:OE1	2.20	0.41
1:F:241:ILE:HD13	1:G:220:LEU:CB	2.50	0.41
1:D:238:LYS:HZ2	1:D:238:LYS:HB2	1.86	0.41
1:B:238:LYS:HZ3	1:B:238:LYS:HB2	1.86	0.41
1:H:71:PHE:HE1	1:H:122:VAL:HB	1.84	0.41
1:E:88:VAL:HG23	1:E:124:ALA:O	2.20	0.41
1:E:153:PHE:CE1	1:E:155:ALA:HA	2.56	0.41
1:H:361:ARG:HH11	1:H:361:ARG:HG2	1.85	0.41
1:B:369:TYR:O	1:B:370:LEU:C	2.58	0.41
1:A:199:ASP:OD1	1:A:200:VAL:N	2.53	0.41
1:D:203:ALA:O	1:D:214:ARG:NH1	2.53	0.41
1:B:82:PRO:HD2	1:B:358:GLU:CG	2.46	0.41
1:H:209:PRO:HD3	1:H:284:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:278:ALA:HB2	1:H:312:LEU:HD12	2.03	0.41
1:F:136:GLU:OE1	1:F:193:ARG:NH1	2.54	0.41
1:E:104:HIS:H	1:E:107:ASN:HD22	1.68	0.41
1:A:82:PRO:HD2	1:A:358:GLU:HG3	2.01	0.41
1:C:96:LEU:CD1	1:C:110:ALA:HB3	2.50	0.41
1:D:188:SER:C	1:D:189:ILE:HG13	2.41	0.41
1:D:177:ASN:HA	1:D:192:HIS:O	2.21	0.41
1:A:96:LEU:CD1	1:A:110:ALA:HB3	2.51	0.41
1:E:209:PRO:HD3	1:E:284:TRP:CD1	2.55	0.41
1:D:153:PHE:CE1	1:D:155:ALA:HA	2.55	0.41
1:G:199:ASP:OD1	1:G:200:VAL:N	2.54	0.41
1:E:278:ALA:HB2	1:E:312:LEU:HD12	2.02	0.41
1:D:283:LYS:HB3	1:E:287:LYS:HG3	2.03	0.41
1:H:359:SER:HB2	1:H:363:ARG:NH1	2.35	0.41
1:H:311:PHE:O	1:H:314:PRO:HD2	2.21	0.41
1:H:100:LYS:HG3	1:H:101:ASN:N	2.36	0.41
1:B:100:LYS:HG3	1:B:101:ASN:N	2.35	0.41
1:F:257:ARG:NE	1:F:257:ARG:HA	2.36	0.41
1:F:88:VAL:HG23	1:F:124:ALA:O	2.20	0.41
1:E:28:GLN:OE1	1:F:26:LYS:CE	2.69	0.41
1:B:147:TYR:H	1:B:147:TYR:HD1	1.67	0.41
1:E:1:MET:HA	1:E:21:ASP:OD2	2.20	0.41
1:B:203:ALA:O	1:B:214:ARG:NH1	2.54	0.41
1:G:324:ALA:HB1	1:G:325:PRO:HD2	2.03	0.41
1:F:72:VAL:HG12	1:F:338:LEU:HD22	2.03	0.41
1:A:24:MET:CE	1:B:24:MET:HE3	2.51	0.41
1:H:80:PRO:O	1:H:81:ILE:HG23	2.21	0.41
1:A:16:LEU:HD11	1:A:54:ALA:HA	2.03	0.41
1:A:169:MET:O	1:A:171:LYS:HG3	2.20	0.41
1:G:88:VAL:HG12	1:G:93:ILE:CD1	2.37	0.41
1:D:255:ASP:OD1	1:D:257:ARG:HB2	2.21	0.41
1:C:223:LEU:O	1:C:227:CYS:HB2	2.21	0.41
1:A:141:VAL:HG13	1:H:250:TYR:CE2	2.56	0.41
1:E:144:HIS:CE1	1:E:146:ASN:ND2	2.84	0.41
1:G:82:PRO:CD	1:G:358:GLU:HG3	2.48	0.41
1:A:186:GLY:HA2	1:A:211:THR:HG21	2.03	0.41
1:A:211:THR:HB	1:A:212:PRO:CD	2.51	0.41
1:F:361:ARG:O	1:F:365:ARG:NE	2.53	0.41
1:A:147:TYR:H	1:A:147:TYR:HD1	1.67	0.41
1:C:199:ASP:OD1	1:C:200:VAL:N	2.53	0.41
1:F:345:VAL:CG1	1:F:352:PRO:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:O	1:D:120:THR:HG21	2.21	0.41
1:B:177:ASN:HA	1:B:192:HIS:O	2.20	0.41
1:G:27:MET:C	1:G:27:MET:SD	2.99	0.41
1:A:27:MET:SD	1:A:27:MET:C	2.99	0.41
1:E:80:PRO:HB2	1:E:362:TRP:CZ3	2.56	0.41
1:C:100:LYS:HG3	1:C:101:ASN:N	2.36	0.41
1:H:333:ASN:HD22	1:H:336:LYS:HB2	1.86	0.41
1:E:307:HIS:HA	1:E:309:LYS:HE3	2.02	0.41
1:E:96:LEU:CD1	1:E:110:ALA:HB3	2.49	0.41
1:G:96:LEU:CD1	1:G:110:ALA:HB3	2.51	0.41
1:G:251:LEU:C	1:G:253:THR:H	2.25	0.40
1:E:203:ALA:O	1:E:214:ARG:NH1	2.54	0.40
1:G:211:THR:HB	1:G:212:PRO:CD	2.51	0.40
1:G:311:PHE:C	1:G:314:PRO:HD2	2.41	0.40
1:G:238:LYS:HB2	1:G:238:LYS:HZ3	1.85	0.40
1:A:196:ARG:HH22	1:A:365:ARG:NH2	2.19	0.40
1:F:278:ALA:HB2	1:F:312:LEU:HD12	2.03	0.40
1:F:20:GLU:O	1:F:21:ASP:HB2	2.21	0.40
1:A:144:HIS:CE1	1:A:146:ASN:HD22	2.38	0.40
1:C:275:ARG:HA	1:C:315:TRP:CZ3	2.56	0.40
1:E:256:ALA:O	1:E:260:VAL:HG23	2.21	0.40
1:D:77:LEU:HD21	1:D:204:LEU:HD12	2.01	0.40
1:G:203:ALA:O	1:G:214:ARG:NH1	2.54	0.40
1:F:224:VAL:CG2	1:G:223:LEU:HD21	2.51	0.40
1:C:129:PRO:C	1:C:131:VAL:H	2.24	0.40
1:A:294:GLY:O	1:A:296:VAL:N	2.53	0.40
1:H:268:GLU:OE1	1:H:268:GLU:HA	2.21	0.40
1:C:104:HIS:ND1	1:C:105:ALA:N	2.70	0.40
1:F:283:LYS:CE	1:G:287:LYS:HE2	2.46	0.40
1:E:189:ILE:CD1	1:E:284:TRP:HB2	2.51	0.40
1:H:55:ARG:NH1	1:H:55:ARG:HG2	2.32	0.40
1:G:186:GLY:HA2	1:G:211:THR:HG21	2.03	0.40
1:H:311:PHE:C	1:H:314:PRO:HD2	2.41	0.40
1:F:240:ARG:NH1	1:F:244:ASN:ND2	2.68	0.40
1:C:88:VAL:HG23	1:C:124:ALA:O	2.20	0.40
1:C:345:VAL:CG1	1:C:352:PRO:HG3	2.51	0.40
1:B:294:GLY:O	1:B:296:VAL:N	2.55	0.40
1:G:268:GLU:OE1	1:G:268:GLU:HA	2.21	0.40
1:E:369:TYR:HB3	1:E:370:LEU:CD1	2.48	0.40
1:E:161:VAL:HG23	1:E:162:ALA:N	2.37	0.40
1:G:79:ASP:O	1:G:81:ILE:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ALA:HB2	1:B:312:LEU:HD12	2.03	0.40
1:A:333:ASN:OD1	1:A:336:LYS:HB2	2.22	0.40
1:B:96:LEU:CD1	1:B:110:ALA:HB3	2.52	0.40
1:D:64:SER:C	1:D:66:SER:N	2.74	0.40
1:F:324:ALA:HB1	1:F:325:PRO:HD2	2.02	0.40
1:F:16:LEU:HD11	1:F:54:ALA:HA	2.02	0.40
1:D:345:VAL:CG1	1:D:352:PRO:HG3	2.52	0.40
1:D:104:HIS:NE2	4:D:381:CIT:H21	2.36	0.40
1:F:223:LEU:O	1:F:227:CYS:HB2	2.22	0.40
1:D:153:PHE:N	1:D:153:PHE:CD2	2.90	0.40
1:B:369:TYR:O	1:B:371:ASP:N	2.55	0.40
1:H:333:ASN:ND2	1:H:336:LYS:CB	2.84	0.40
1:A:92:MET:HB2	1:A:355:TYR:CD2	2.57	0.40
1:C:59:GLU:C	1:C:61:THR:H	2.25	0.40
1:H:129:PRO:O	1:H:132:VAL:HG23	2.22	0.40
1:G:177:ASN:HA	1:G:192:HIS:O	2.21	0.40
1:D:315:TRP:O	1:D:319:ARG:HG3	2.21	0.40
1:A:315:TRP:O	1:A:319:ARG:HG3	2.21	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	371/375 (99%)	325 (88%)	39 (10%)	7 (2%)	10	43
1	B	369/375 (98%)	326 (88%)	39 (11%)	4 (1%)	17	58
1	C	369/375 (98%)	325 (88%)	38 (10%)	6 (2%)	12	48
1	D	371/375 (99%)	327 (88%)	41 (11%)	3 (1%)	24	66
1	E	369/375 (98%)	325 (88%)	40 (11%)	4 (1%)	17	58
1	F	370/375 (99%)	325 (88%)	43 (12%)	2 (0%)	34	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	371/375 (99%)	322 (87%)	45 (12%)	4 (1%)	17	58
1	H	370/375 (99%)	326 (88%)	41 (11%)	3 (1%)	24	66
All	All	2960/3000 (99%)	2601 (88%)	326 (11%)	33 (1%)	17	58

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	LEU
1	H	60	GLU
1	A	39	ARG
1	A	243	GLY
1	C	245	GLY
1	C	368	SER
1	E	39	ARG
1	F	39	ARG
1	H	39	ARG
1	A	308	GLU
1	C	60	GLU
1	C	233	THR
1	C	267	ASP
1	D	372	GLY
1	E	233	THR
1	G	39	ARG
1	G	233	THR
1	A	233	THR
1	B	205	ASP
1	B	233	THR
1	B	308	GLU
1	C	308	GLU
1	D	233	THR
1	E	308	GLU
1	F	233	THR
1	G	60	GLU
1	G	205	ASP
1	H	233	THR
1	A	205	ASP
1	A	267	ASP
1	A	333	ASN
1	D	205	ASP
1	E	330	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	313/315 (99%)	306 (98%)	7 (2%)	60	88
1	B	312/315 (99%)	307 (98%)	5 (2%)	70	92
1	C	312/315 (99%)	308 (99%)	4 (1%)	76	93
1	D	313/315 (99%)	307 (98%)	6 (2%)	65	90
1	E	312/315 (99%)	306 (98%)	6 (2%)	65	90
1	F	312/315 (99%)	303 (97%)	9 (3%)	50	84
1	G	313/315 (99%)	308 (98%)	5 (2%)	70	92
1	H	312/315 (99%)	306 (98%)	6 (2%)	65	90
All	All	2499/2520 (99%)	2451 (98%)	48 (2%)	65	90

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	137	ASP
1	A	238	LYS
1	A	257	ARG
1	A	284	TRP
1	A	333	ASN
1	A	365	ARG
1	B	48	GLU
1	B	137	ASP
1	B	153	PHE
1	B	238	LYS
1	B	284	TRP
1	C	39	ARG
1	C	238	LYS
1	C	284	TRP
1	C	369	TYR
1	D	39	ARG
1	D	48	GLU
1	D	136	GLU

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Mol	Chain	Res	Type
1	D	153	PHE
1	D	238	LYS
1	D	361	ARG
1	E	153	PHE
1	E	238	LYS
1	E	257	ARG
1	E	258	GLU
1	E	333	ASN
1	E	369	TYR
1	F	23	ARG
1	F	137	ASP
1	F	147	TYR
1	F	153	PHE
1	F	172	ARG
1	F	238	LYS
1	F	257	ARG
1	F	284	TRP
1	F	333	ASN
1	G	60	GLU
1	G	153	PHE
1	G	238	LYS
1	G	333	ASN
1	G	371	ASP
1	H	23	ARG
1	H	153	PHE
1	H	238	LYS
1	H	257	ARG
1	H	284	TRP
1	H	361	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	146	ASN
1	A	222	GLN
1	A	265	GLN
1	A	333	ASN
1	B	144	HIS
1	B	222	GLN
1	B	265	GLN
1	B	307	HIS

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Mol	Chain	Res	Type
1	B	333	ASN
1	C	28	GLN
1	C	56	GLN
1	C	114	HIS
1	C	144	HIS
1	C	146	ASN
1	C	222	GLN
1	C	244	ASN
1	C	265	GLN
1	C	333	ASN
1	D	28	GLN
1	D	146	ASN
1	D	222	GLN
1	D	265	GLN
1	E	56	GLN
1	E	114	HIS
1	E	144	HIS
1	E	222	GLN
1	E	265	GLN
1	E	333	ASN
1	F	114	HIS
1	F	146	ASN
1	F	148	GLN
1	F	222	GLN
1	F	333	ASN
1	G	28	GLN
1	G	56	GLN
1	G	146	ASN
1	G	222	GLN
1	G	244	ASN
1	G	265	GLN
1	G	333	ASN
1	H	28	GLN
1	H	56	GLN
1	H	114	HIS
1	H	144	HIS
1	H	244	ASN
1	H	333	ASN

### 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](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	GOL	A	395	-	5,5,5	4.67	5 (100%)	5,5,5	5.38	4 (80%)
5	GOL	B	394	-	5,5,5	4.70	5 (100%)	5,5,5	5.38	4 (80%)
3	PO4	B	402	-	4,4,4	0.73	0	6,6,6	0.30	0
5	GOL	C	392	-	5,5,5	4.67	5 (100%)	5,5,5	5.38	4 (80%)
4	CIT	D	381	-	3,12,12	2.68	1 (33%)	3,17,17	3.36	2 (66%)
4	CIT	D	384	-	3,12,12	2.78	1 (33%)	3,17,17	2.62	2 (66%)
5	GOL	D	393	-	5,5,5	4.77	5 (100%)	5,5,5	5.54	4 (80%)
3	PO4	E	401	-	4,4,4	0.70	0	6,6,6	0.30	0
3	PO4	E	405	-	4,4,4	0.72	0	6,6,6	0.30	0
5	GOL	F	391	-	5,5,5	4.65	5 (100%)	5,5,5	5.29	4 (80%)
3	PO4	F	403	-	4,4,4	0.73	0	6,6,6	0.30	0
4	CIT	G	382	-	3,12,12	2.59	1 (33%)	3,17,17	3.18	2 (66%)
4	CIT	G	383	-	3,12,12	2.72	1 (33%)	3,17,17	2.80	2 (66%)
3	PO4	H	404	-	4,4,4	0.75	0	6,6,6	0.30	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
5	GOL	A	395	-	-	0/4/4/4	0/0/0/0
5	GOL	B	394	-	-	0/4/4/4	0/0/0/0
3	PO4	B	402	-	-	0/0/0/0	0/0/0/0
5	GOL	C	392	-	-	0/4/4/4	0/0/0/0
4	CIT	D	381	-	-	0/6/16/16	0/0/0/0
4	CIT	D	384	-	-	0/6/16/16	0/0/0/0
5	GOL	D	393	-	-	0/4/4/4	0/0/0/0
3	PO4	E	401	-	-	0/0/0/0	0/0/0/0
3	PO4	E	405	-	-	0/0/0/0	0/0/0/0
5	GOL	F	391	-	-	0/4/4/4	0/0/0/0
3	PO4	F	403	-	-	0/0/0/0	0/0/0/0
4	CIT	G	382	-	-	0/6/16/16	0/0/0/0
4	CIT	G	383	-	-	0/6/16/16	0/0/0/0
3	PO4	H	404	-	-	0/0/0/0	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	393	GOL	C3-C2	-7.84	1.22	1.52
5	A	395	GOL	C3-C2	-7.63	1.23	1.52
5	C	392	GOL	C3-C2	-7.58	1.23	1.52
5	B	394	GOL	C3-C2	-7.58	1.23	1.52
5	F	391	GOL	C3-C2	-7.56	1.23	1.52
5	F	391	GOL	C1-C2	-3.55	1.38	1.52
5	B	394	GOL	C1-C2	-3.37	1.39	1.52
5	C	392	GOL	C1-C2	-3.33	1.39	1.52
5	A	395	GOL	C1-C2	-3.33	1.39	1.52
5	D	393	GOL	O2-C2	-3.25	1.33	1.43
5	D	393	GOL	C1-C2	-3.17	1.40	1.52
5	A	395	GOL	O2-C2	-3.09	1.34	1.43
5	B	394	GOL	O2-C2	-3.09	1.34	1.43
5	C	392	GOL	O2-C2	-2.97	1.34	1.43
5	F	391	GOL	O2-C2	-2.83	1.35	1.43
5	A	395	GOL	O3-C3	3.21	1.56	1.42
5	D	393	GOL	O3-C3	3.23	1.56	1.42
5	C	392	GOL	O3-C3	3.37	1.56	1.42
5	B	394	GOL	O3-C3	3.38	1.56	1.42
5	F	391	GOL	O3-C3	3.45	1.57	1.42
4	G	382	CIT	O7-C3	4.17	1.49	1.43
5	F	391	GOL	O1-C1	4.29	1.60	1.42
4	G	383	CIT	O7-C3	4.30	1.50	1.43
4	D	384	CIT	O7-C3	4.42	1.50	1.43
4	D	381	CIT	O7-C3	4.47	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	395	GOL	O1-C1	4.47	1.61	1.42
5	C	392	GOL	O1-C1	4.48	1.61	1.42
5	B	394	GOL	O1-C1	4.54	1.61	1.42
5	D	393	GOL	O1-C1	4.63	1.62	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	393	GOL	C3-C2-C1	-2.81	100.10	111.12
5	A	395	GOL	C3-C2-C1	-2.54	101.15	111.12
5	F	391	GOL	C3-C2-C1	-2.48	101.39	111.12
5	B	394	GOL	C3-C2-C1	-2.48	101.41	111.12
5	C	392	GOL	C3-C2-C1	-2.44	101.56	111.12
4	D	384	CIT	C3-C4-C5	2.22	118.50	114.96
4	G	383	CIT	C3-C4-C5	2.29	118.62	114.96
4	D	381	CIT	C3-C4-C5	2.76	119.38	114.96
5	F	391	GOL	O1-C1-C2	3.06	125.04	110.18
5	D	393	GOL	O1-C1-C2	3.24	125.89	110.18
5	B	394	GOL	O1-C1-C2	3.25	125.93	110.18
5	C	392	GOL	O1-C1-C2	3.25	125.96	110.18
5	A	395	GOL	O1-C1-C2	3.28	126.10	110.18
4	G	382	CIT	C3-C4-C5	3.61	120.74	114.96
4	D	384	CIT	C3-C2-C1	3.95	121.28	114.96
4	G	382	CIT	C3-C2-C1	4.16	121.61	114.96
5	C	392	GOL	O2-C2-C3	4.27	128.21	108.65
4	G	383	CIT	C3-C2-C1	4.28	121.79	114.96
5	F	391	GOL	O2-C2-C3	4.31	128.39	108.65
5	B	394	GOL	O2-C2-C3	4.39	128.77	108.65
5	A	395	GOL	O2-C2-C3	4.46	129.11	108.65
5	D	393	GOL	O2-C2-C3	4.81	130.72	108.65
4	D	381	CIT	C3-C2-C1	5.02	122.98	114.96
5	F	391	GOL	O3-C3-C2	10.29	160.08	110.18
5	A	395	GOL	O3-C3-C2	10.37	160.50	110.18
5	B	394	GOL	O3-C3-C2	10.42	160.73	110.18
5	C	392	GOL	O3-C3-C2	10.47	160.98	110.18
5	D	393	GOL	O3-C3-C2	10.58	161.50	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	381	CIT	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	373/375 (99%)	0.12	16 (4%)	39 16	14, 49, 111, 139	0
1	B	371/375 (98%)	0.24	12 (3%)	51 23	10, 52, 117, 136	0
1	C	371/375 (98%)	0.17	13 (3%)	48 21	15, 47, 105, 138	0
1	D	373/375 (99%)	0.11	14 (3%)	44 18	18, 39, 109, 140	0
1	E	371/375 (98%)	0.03	4 (1%)	82 58	20, 43, 101, 135	0
1	F	372/375 (99%)	0.10	9 (2%)	62 32	23, 49, 105, 143	0
1	G	373/375 (99%)	0.15	16 (4%)	39 16	23, 46, 113, 142	0
1	H	372/375 (99%)	0.18	14 (3%)	44 18	21, 54, 117, 146	0
All	All	2976/3000 (99%)	0.14	98 (3%)	50 22	10, 48, 111, 146	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	242	VAL	8.4
1	A	373	ILE	7.5
1	B	237	MET	5.9
1	G	229	SER	5.8
1	D	373	ILE	5.5
1	C	369	TYR	5.2
1	B	241	ILE	4.9
1	H	237	MET	4.9
1	D	237	MET	4.8
1	G	373	ILE	4.7
1	G	221	THR	4.6
1	E	369	TYR	4.5
1	G	225	ASP	4.4
1	C	237	MET	4.3
1	D	372	GLY	4.3
1	C	147	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	147	TYR	4.1
1	G	231	LYS	4.1
1	G	242	VAL	4.1
1	C	232	PHE	4.0
1	H	227	CYS	4.0
1	H	224	VAL	3.9
1	B	236	GLU	3.9
1	D	241	ILE	3.9
1	A	147	TYR	3.9
1	A	372	GLY	3.9
1	G	244	ASN	3.9
1	G	241	ILE	3.8
1	H	75	GLY	3.8
1	D	243	GLY	3.8
1	A	242	VAL	3.7
1	D	147	TYR	3.7
1	B	369	TYR	3.7
1	B	368	SER	3.5
1	B	225	ASP	3.4
1	A	369	TYR	3.4
1	H	369	TYR	3.4
1	C	229	SER	3.3
1	H	147	TYR	3.3
1	G	237	MET	3.2
1	B	221	THR	3.2
1	A	231	LYS	3.2
1	H	272	ARG	3.1
1	F	232	PHE	3.1
1	F	369	TYR	3.1
1	F	229	SER	3.0
1	C	75	GLY	3.0
1	D	236	GLU	3.0
1	G	236	GLU	2.8
1	B	147	TYR	2.8
1	F	225	ASP	2.8
1	C	371	ASP	2.8
1	A	232	PHE	2.7
1	B	104	HIS	2.7
1	A	236	GLU	2.7
1	F	224	VAL	2.7
1	C	265	GLN	2.7
1	C	225	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	244	ASN	2.6
1	B	371	ASP	2.6
1	D	220	LEU	2.6
1	E	228	PHE	2.6
1	A	241	ILE	2.6
1	E	147	TYR	2.6
1	F	237	MET	2.5
1	G	371	ASP	2.5
1	F	147	TYR	2.5
1	E	246	GLY	2.5
1	G	215	SER	2.4
1	A	265	GLN	2.4
1	D	235	GLU	2.4
1	F	236	GLU	2.4
1	C	222	GLN	2.4
1	A	75	GLY	2.3
1	D	222	GLN	2.3
1	A	221	THR	2.3
1	H	23	ARG	2.2
1	H	231	LYS	2.2
1	G	265	GLN	2.2
1	H	221	THR	2.2
1	C	226	LEU	2.2
1	C	39	ARG	2.2
1	H	370	LEU	2.2
1	H	220	LEU	2.1
1	D	225	ASP	2.1
1	B	41	GLN	2.1
1	H	236	GLU	2.1
1	A	237	MET	2.1
1	A	367	ASP	2.1
1	F	227	CYS	2.1
1	A	230	GLY	2.1
1	C	230	GLY	2.1
1	B	218	LEU	2.1
1	D	230	GLY	2.0
1	H	225	ASP	2.0
1	G	238	LYS	2.0
1	A	229	SER	2.0
1	G	232	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
5	GOL	C	392	6/6	0.64	0.42	4.02	40,43,44,44	0
5	GOL	A	395	6/6	0.32	0.46	3.57	68,71,71,71	0
5	GOL	F	391	6/6	0.67	0.34	2.24	56,58,59,59	0
4	CIT	D	384	13/13	0.62	0.32	1.89	89,91,92,92	0
4	CIT	G	383	13/13	0.62	0.37	1.34	88,92,95,96	0
4	CIT	D	381	13/13	0.51	0.31	1.26	78,80,81,81	0
4	CIT	G	382	13/13	0.70	0.31	1.13	67,68,69,70	0
3	PO4	E	405	5/5	0.81	0.25	0.80	97,98,98,99	0
5	GOL	D	393	6/6	0.75	0.27	0.41	43,44,46,49	0
3	PO4	E	401	5/5	0.91	0.23	0.38	76,76,77,78	0
5	GOL	B	394	6/6	0.75	0.27	0.23	54,54,55,55	0
3	PO4	F	403	5/5	0.82	0.22	0.10	98,99,99,100	0
3	PO4	B	402	5/5	0.91	0.21	-0.13	83,83,83,84	0
3	PO4	H	404	5/5	0.87	0.20	-0.44	76,77,78,78	0
2	NA	D	380	1/1	0.92	0.09	-3.87	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.