



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:32 am GMT

PDB ID : 1K93  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin  
Authors : Drum, C.L.; Yan, S.-Z.; Bard, J.; Shen, Y.-Q.; Lu, D.; Soelaiman, S.; Grabarek, Z.; Bohm, A.; Tang, W.-J.  
Deposited on : 2001-10-26  
Resolution : 2.95 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

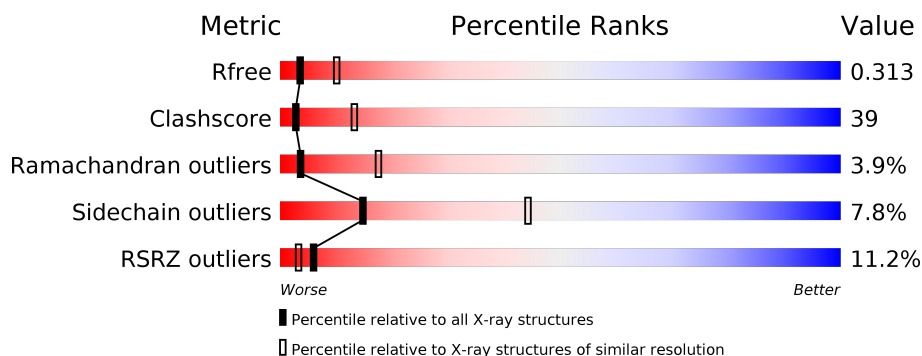
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div>3%</div> <div>49%</div> <div>38%</div> <div>8%</div> <div>5%</div> </div>
1	B	510	<div> <div>8%</div> <div>32%</div> <div>49%</div> <div>9%</div> <div>8%</div> </div>
1	C	510	<div> <div>6%</div> <div>48%</div> <div>43%</div> <div>7%</div> </div>
2	D	144	<div> <div>26%</div> <div>43%</div> <div>52%</div> </div>
2	E	144	<div> <div>33%</div> <div>38%</div> <div>57%</div> </div>
2	F	144	<div> <div>26%</div> <div>35%</div> <div>60%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15241 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

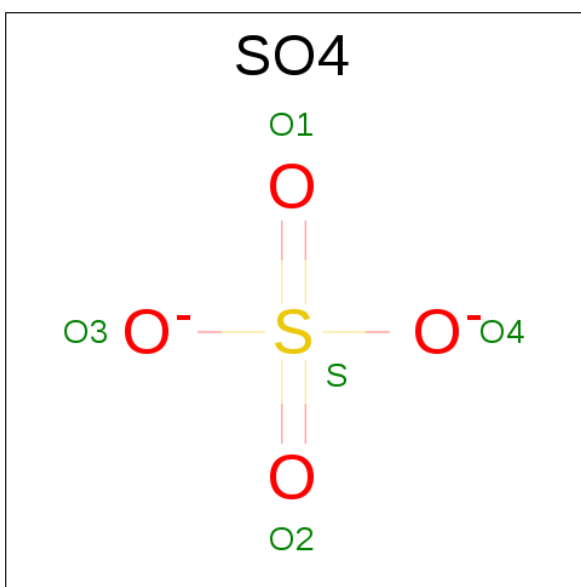
- Molecule 1 is a protein called CALMODULIN-SENSITIVE ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	65	0	0
			3952	2528	673	748	3			
1	B	467	Total	C	N	O	S	113	0	0
			3804	2437	644	720	3			
1	C	503	Total	C	N	O	S	166	0	0
			4094	2616	696	779	3			

- Molecule 2 is a protein called CALMODULIN.

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

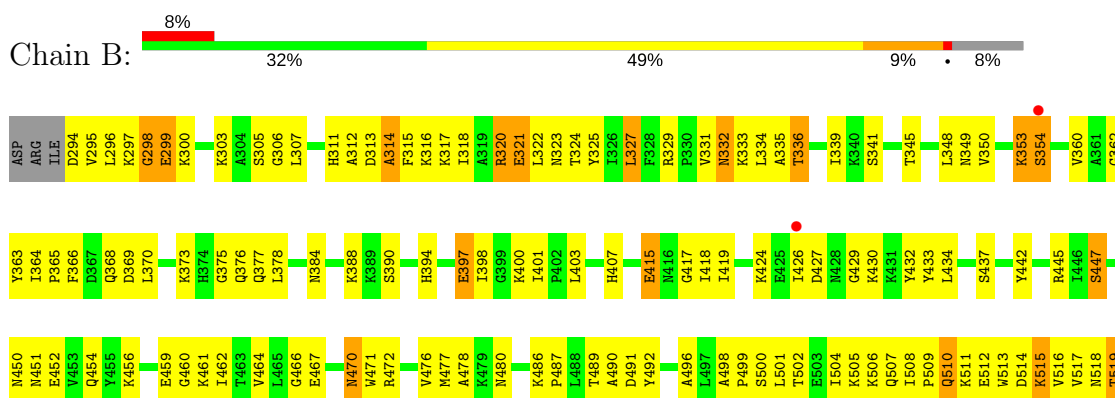
### 3 Residue-property plots

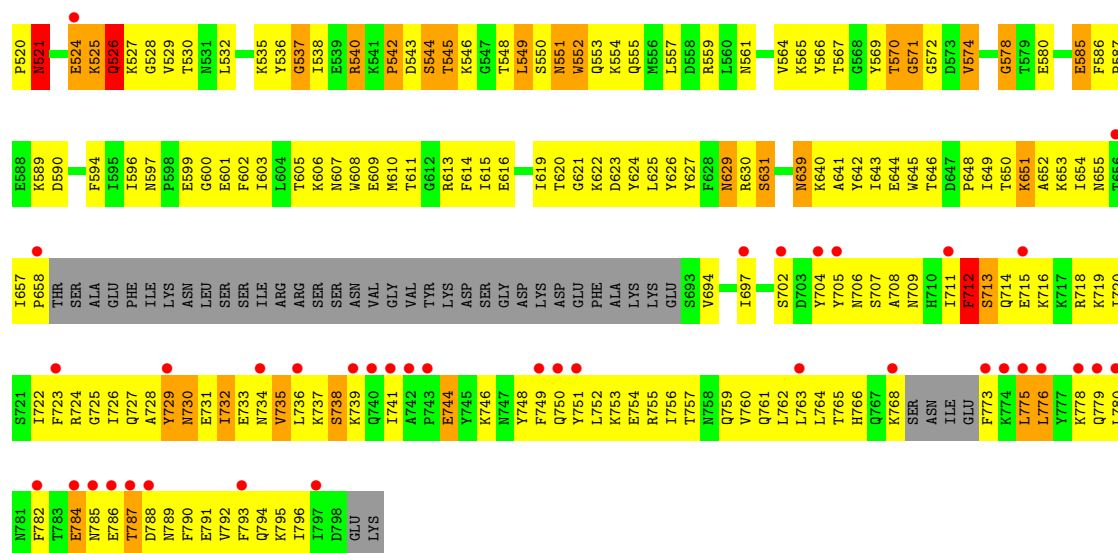
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: CALMODULIN-SENSITIVE ADENYLATE CYCLASE

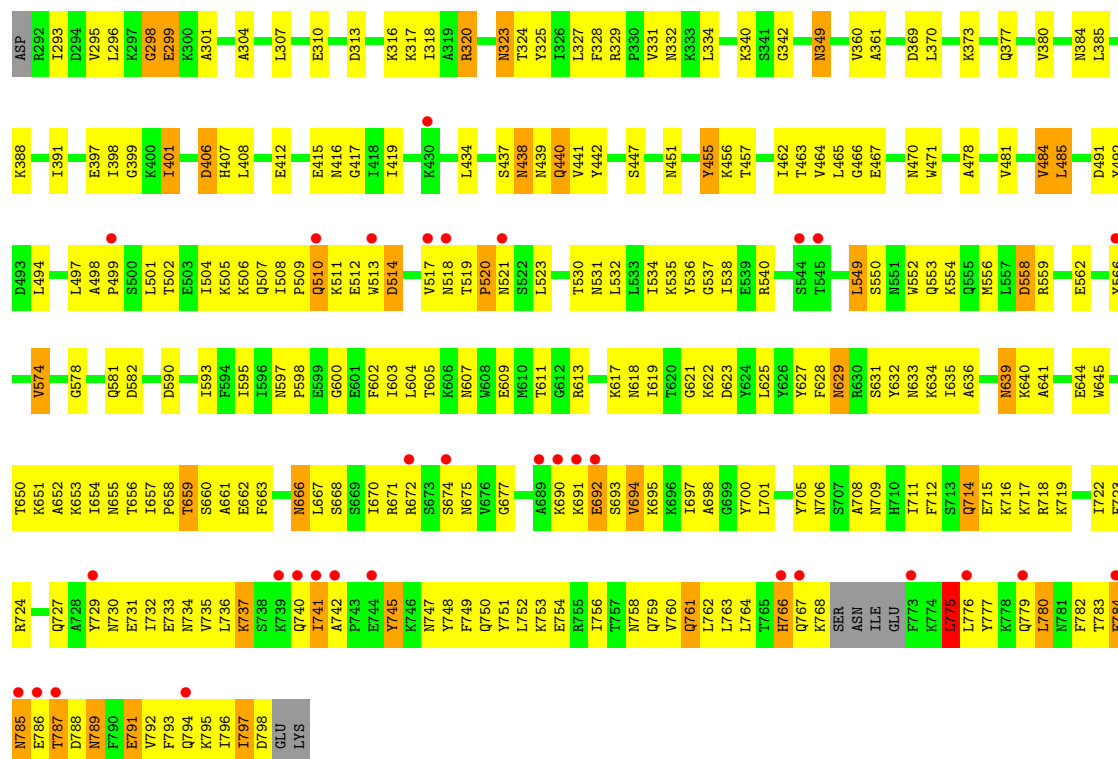


#### • Molecule 1: CALMODULIN-SENSITIVE ADENYLATE CYCLASE

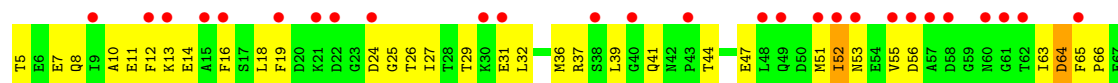
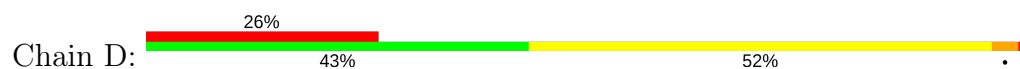


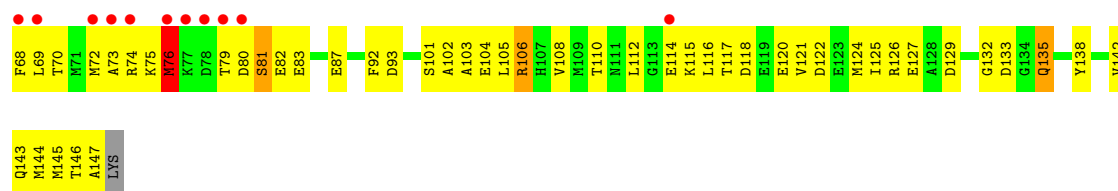


• Molecule 1: CALMODULIN-SENSITIVE ADENYLATE CYCLASE

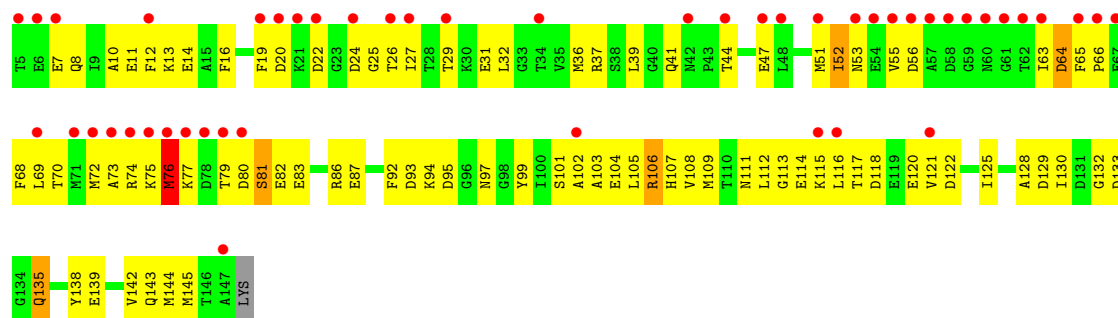


• Molecule 2: CALMODULIN

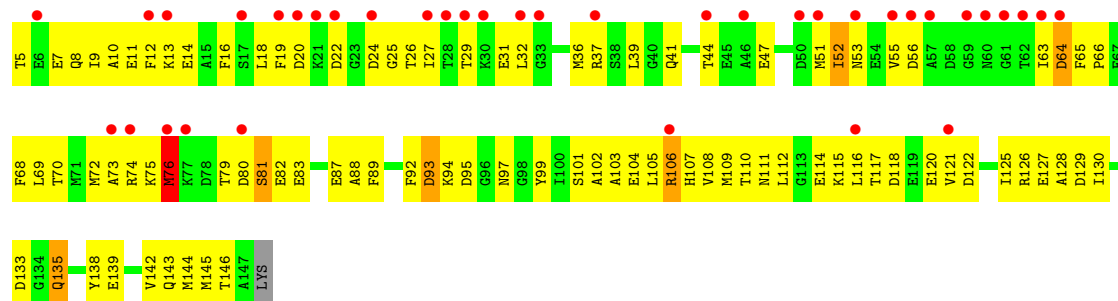




• Molecule 2: CALMODULIN



• Molecule 2: CALMODULIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.73Å 167.31Å 344.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.95 30.00 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.95) 97.7 (30.00-2.94)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.278 , 0.315 0.278 , 0.313	Depositor DCC
$R_{free}$ test set	7056 reflections (10.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15241	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: CA, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.57	1/4027 (0.0%)	0.87	17/5419 (0.3%)
1	B	0.67	4/3878 (0.1%)	0.85	6/5221 (0.1%)
1	C	0.55	0/4172	0.79	8/5613 (0.1%)
2	D	0.40	0/1137	0.66	2/1527 (0.1%)
2	E	0.45	0/1137	0.67	2/1527 (0.1%)
2	F	0.41	0/1137	0.77	3/1527 (0.2%)
All	All	0.56	5/15488 (0.0%)	0.81	38/20834 (0.2%)

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	C	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	SER	CB-OG	9.02	1.53	1.42
1	B	525	LYS	CE-NZ	7.07	1.66	1.49
1	B	354	SER	CA-CB	6.45	1.62	1.52
1	A	470	ASN	C-N	-5.49	1.21	1.34
1	B	525	LYS	C-O	5.24	1.33	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	106	ARG	NE-CZ-NH1	-13.77	113.41	120.30
2	F	106	ARG	NE-CZ-NH2	13.70	127.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ARG	NE-CZ-NH1	-11.75	114.43	120.30
1	C	613	ARG	NE-CZ-NH2	-11.48	114.56	120.30
1	A	613	ARG	NE-CZ-NH2	11.09	125.84	120.30
1	C	613	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	A	784	GLU	N-CA-CB	10.05	128.70	110.60
1	C	320	ARG	NE-CZ-NH2	9.98	125.29	120.30
1	C	320	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	A	320	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	785	ASN	C-N-CA	-9.08	99.00	121.70
1	A	320	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	B	521	ASN	N-CA-C	8.86	134.91	111.00
1	B	525	LYS	N-CA-C	-8.48	88.10	111.00
1	C	785	ASN	C-N-CA	-7.74	102.36	121.70
1	A	470	ASN	C-N-CA	-7.73	102.37	121.70
1	A	785	ASN	CA-C-N	7.65	134.03	117.20
1	A	785	ASN	O-C-N	-7.16	111.24	122.70
1	B	521	ASN	C-N-CA	-7.13	103.88	121.70
1	A	784	GLU	C-N-CA	-7.12	103.90	121.70
1	A	785	ASN	N-CA-C	6.97	129.81	111.00
2	E	106	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	470	ASN	CA-C-N	6.85	132.27	117.20
2	E	106	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	784	GLU	N-CA-C	-6.64	93.07	111.00
2	F	106	ARG	CD-NE-CZ	6.64	132.90	123.60
2	D	106	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	693	SER	N-CA-CB	-6.46	100.81	110.50
1	B	549	LEU	CA-CB-CG	6.41	130.05	115.30
2	D	106	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	785	ASN	N-CA-C	5.87	126.86	111.00
1	A	470	ASN	N-CA-C	5.78	126.59	111.00
1	C	613	ARG	CD-NE-CZ	5.44	131.21	123.60
1	A	471	TRP	N-CA-C	-5.39	96.46	111.00
1	A	613	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	470	ASN	N-CA-CB	5.22	119.99	110.60
1	B	370	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	785	ASN	CA-CB-CG	-5.17	102.02	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	566	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	766	HIS	Mainchain

## 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	3952	0	3999	282	0
1	B	3804	0	3833	380	0
1	C	4094	0	4134	287	0
2	D	1125	0	1049	82	0
2	E	1125	0	1049	77	0
2	F	1125	0	1049	90	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
All	All	15241	0	15113	1150	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 39.

All (1150) 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:B:616:GLU:HA	1:B:620:THR:HG22	1.31	1.11
1:B:327:LEU:HD22	1:B:496:ALA:HB3	1.35	1.07
1:B:726:ILE:HA	1:B:729:TYR:HB2	1.35	1.03
2:F:19:PHE:HD1	2:F:19:PHE:O	1.42	1.02
1:C:714:GLN:HA	1:C:714:GLN:HE21	1.25	1.01
1:A:463:THR:HG22	1:A:465:LEU:H	1.24	0.99
1:B:605:THR:HG21	1:B:611:THR:OG1	1.62	0.99
1:B:324:THR:HG22	1:B:499:PRO:HA	1.44	0.99
1:C:463:THR:HG22	1:C:465:LEU:H	1.25	0.99
1:C:519:THR:OG1	1:C:520:PRO:HD2	1.62	0.98
1:B:629:ASN:HD22	1:B:631:SER:H	0.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LYS:HA	1:B:535:LYS:HE2	1.44	0.97
1:A:456:LYS:HD3	1:A:471:TRP:CD1	2.00	0.95
2:F:19:PHE:CD1	2:F:19:PHE:O	2.19	0.95
1:B:551:ASN:ND2	1:B:551:ASN:H	1.63	0.95
1:B:320:ARG:HB3	1:B:320:ARG:HH21	1.27	0.94
1:B:489:THR:HG22	1:B:490:ALA:H	1.31	0.94
1:A:714:GLN:HE21	1:A:714:GLN:HA	1.31	0.94
1:B:551:ASN:HD22	1:B:551:ASN:H	1.04	0.93
1:B:360:VAL:HG21	1:B:365:PRO:HG3	1.51	0.93
1:A:349:ASN:HD22	1:A:349:ASN:H	1.17	0.93
1:C:629:ASN:HD22	1:C:631:SER:H	1.04	0.93
1:A:789:ASN:N	1:A:789:ASN:HD22	1.67	0.93
2:E:19:PHE:CD1	2:E:19:PHE:O	2.21	0.93
2:E:19:PHE:HD1	2:E:19:PHE:O	1.49	0.93
1:B:353:LYS:H	1:B:368:GLN:HE22	0.92	0.92
1:A:629:ASN:HD22	1:A:631:SER:H	1.15	0.92
1:C:629:ASN:ND2	1:C:631:SER:H	1.71	0.89
2:D:19:PHE:O	2:D:19:PHE:HD1	1.55	0.89
1:B:738:SER:HB3	1:B:741:ILE:HD11	1.53	0.89
1:C:783:THR:HB	1:C:784:GLU:OE1	1.72	0.89
1:C:789:ASN:HD22	1:C:789:ASN:N	1.67	0.89
1:C:633:ASN:HD21	1:C:645:TRP:H	1.20	0.88
1:B:325:TYR:HB2	1:B:498:ALA:HB3	1.54	0.88
1:A:456:LYS:HD3	1:A:471:TRP:HD1	1.35	0.88
1:B:648:PRO:HA	1:B:651:LYS:HB2	1.56	0.88
1:C:523:LEU:HD13	2:F:127:GLU:HB3	1.53	0.87
1:B:793:PHE:HA	1:B:796:ILE:HG12	1.55	0.87
1:C:349:ASN:H	1:C:349:ASN:HD22	1.23	0.87
1:C:509:PRO:HG2	1:C:512:GLU:HB2	1.55	0.87
1:C:295:VAL:HG21	1:C:603:ILE:CG2	2.05	0.86
1:B:525:LYS:O	1:B:528:GLY:N	2.09	0.86
1:B:538:ILE:HD11	1:B:625:LEU:HD11	1.59	0.85
1:B:320:ARG:HB3	1:B:320:ARG:NH2	1.91	0.84
1:C:329:ARG:HD2	1:C:590:ASP:OD2	1.77	0.84
1:B:353:LYS:H	1:B:368:GLN:NE2	1.75	0.84
1:A:456:LYS:HB3	1:A:470:ASN:O	1.78	0.83
1:B:514:ASP:HA	1:B:517:VAL:HG12	1.59	0.82
1:C:663:PHE:O	1:C:667:LEU:HG	1.80	0.82
1:B:366:PHE:HD1	1:B:477:MET:CE	1.93	0.82
1:B:629:ASN:HD21	1:B:631:SER:HB2	1.43	0.81
1:C:694:VAL:HG23	1:C:695:LYS:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:TYR:HA	1:A:780:LEU:HD21	1.62	0.81
1:A:722:ILE:HD13	1:A:764:LEU:HD23	1.62	0.81
1:B:722:ILE:O	1:B:726:ILE:HG13	1.79	0.81
2:F:12:PHE:HD1	2:F:39:LEU:HD21	1.46	0.81
2:D:19:PHE:O	2:D:19:PHE:CD1	2.33	0.81
2:E:12:PHE:HD1	2:E:39:LEU:HD21	1.46	0.81
1:B:306:GLY:O	1:B:336:THR:HB	1.79	0.81
1:C:742:ALA:HB3	1:C:745:TYR:HB2	1.63	0.81
1:C:440:GLN:NE2	1:C:441:VAL:HG23	1.96	0.81
1:B:353:LYS:N	1:B:368:GLN:HE22	1.77	0.80
1:C:722:ILE:HD13	1:C:764:LEU:HD23	1.61	0.80
1:B:320:ARG:CB	1:B:320:ARG:HH21	1.94	0.80
1:A:742:ALA:HB3	1:A:745:TYR:HB2	1.61	0.80
1:A:329:ARG:HD2	1:A:590:ASP:OD2	1.80	0.80
1:C:657:ILE:HG13	1:C:759:GLN:CB	2.12	0.79
1:A:445:ARG:HG3	1:A:471:TRP:CZ2	2.17	0.79
1:B:550:SER:H	1:B:553:GLN:HE21	1.29	0.79
1:B:629:ASN:ND2	1:B:631:SER:HB2	1.98	0.79
1:C:777:TYR:HA	1:C:780:LEU:HD21	1.65	0.79
1:C:775:LEU:HB2	1:C:776:LEU:HD12	1.64	0.79
1:B:520:PRO:HB2	1:B:524:GLU:OE1	1.83	0.79
1:A:659:THR:HG22	1:A:662:GLU:HB3	1.63	0.78
1:B:607:ASN:ND2	1:B:610:MET:H	1.81	0.78
1:A:629:ASN:ND2	1:A:631:SER:H	1.82	0.78
1:A:775:LEU:HB2	1:A:776:LEU:HD12	1.66	0.78
1:B:629:ASN:ND2	1:B:631:SER:H	1.79	0.78
2:D:12:PHE:HD1	2:D:39:LEU:HD21	1.47	0.78
1:B:518:ASN:O	1:B:519:THR:HG22	1.85	0.77
1:B:538:ILE:CD1	1:B:625:LEU:HD11	2.14	0.77
1:C:658:PRO:HG3	1:C:752:LEU:HD22	1.64	0.77
1:A:785:ASN:OD1	1:A:786:GLU:HG2	1.84	0.77
1:C:692:GLU:O	1:C:735:VAL:HG22	1.83	0.77
1:B:525:LYS:O	1:B:526:GLN:C	2.24	0.77
1:B:711:ILE:HG13	1:B:712:PHE:HD1	1.50	0.77
1:A:633:ASN:HD21	1:A:645:TRP:H	1.34	0.76
1:C:697:ILE:HD11	1:C:735:VAL:HG21	1.66	0.76
1:B:335:ALA:HB1	1:B:489:THR:CG2	2.15	0.76
1:B:320:ARG:HG3	1:B:321:GLU:N	2.00	0.76
1:C:380:VAL:HG12	1:C:384:ASN:HD21	1.51	0.76
1:A:523:LEU:HD13	2:D:127:GLU:HB3	1.67	0.76
1:A:445:ARG:NE	1:A:471:TRP:HE1	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ASN:ND2	1:A:641:ALA:H	1.85	0.75
1:B:366:PHE:HD1	1:B:477:MET:HE1	1.51	0.75
1:A:324:THR:HG21	1:A:556:MET:CE	2.17	0.75
1:B:629:ASN:HD22	1:B:631:SER:N	1.80	0.75
1:B:639:ASN:ND2	1:B:641:ALA:H	1.84	0.75
1:B:722:ILE:HG12	1:B:760:VAL:HG13	1.68	0.75
1:B:789:ASN:OD1	1:B:792:VAL:HB	1.87	0.75
1:B:320:ARG:HG3	1:B:321:GLU:H	1.51	0.75
1:C:714:GLN:HA	1:C:714:GLN:NE2	2.01	0.74
1:A:440:GLN:NE2	1:A:441:VAL:HG23	2.01	0.74
1:A:670:ILE:HD12	1:A:745:TYR:CE1	2.22	0.74
1:B:332:ASN:ND2	1:B:334:LEU:H	1.85	0.74
1:B:349:ASN:OD1	1:B:350:VAL:HG23	1.87	0.74
1:A:463:THR:HG22	1:A:465:LEU:N	2.01	0.74
1:C:295:VAL:HG21	1:C:603:ILE:HG22	1.67	0.74
1:C:621:GLY:HA2	2:F:94:LYS:O	1.88	0.74
1:C:761:GLN:HE21	1:C:761:GLN:HA	1.52	0.74
1:C:776:LEU:H	1:C:776:LEU:HD12	1.52	0.74
1:B:654:ILE:HA	1:B:755:ARG:CD	2.17	0.74
1:C:629:ASN:HD22	1:C:631:SER:N	1.84	0.73
1:A:777:TYR:C	1:A:780:LEU:HD11	2.08	0.73
1:C:660:SER:HA	1:C:701:LEU:HD12	1.70	0.73
1:A:780:LEU:HD13	1:A:782:PHE:CZ	2.23	0.73
1:B:711:ILE:HG13	1:B:712:PHE:CD1	2.22	0.73
1:B:362:GLY:O	1:B:489:THR:HG23	1.87	0.73
1:C:780:LEU:HD13	1:C:782:PHE:CZ	2.22	0.73
1:B:366:PHE:HA	1:B:477:MET:HE3	1.68	0.73
1:B:509:PRO:HG2	1:B:512:GLU:HB3	1.68	0.73
1:C:456:LYS:HD3	1:C:471:TRP:CE2	2.24	0.73
1:A:522:SER:OG	2:D:127:GLU:HG3	1.89	0.72
1:A:734:ASN:HA	1:A:737:LYS:HB2	1.71	0.72
1:A:295:VAL:HG23	1:A:604:LEU:O	1.90	0.72
1:C:310:GLU:OE1	1:C:340:LYS:HE3	1.90	0.72
1:C:714:GLN:OE1	2:F:126:ARG:HG2	1.89	0.72
1:B:730:ASN:HA	1:B:733:GLU:HB3	1.70	0.72
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.71	0.72
1:A:295:VAL:HG21	1:A:603:ILE:CG2	2.20	0.72
1:A:715:GLU:O	1:A:719:LYS:HG2	1.89	0.72
1:B:737:LYS:O	1:B:738:SER:C	2.27	0.72
1:A:445:ARG:NE	1:A:471:TRP:NE1	2.39	0.71
1:A:349:ASN:HD22	1:A:349:ASN:N	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HB	1:C:467:GLU:H	1.55	0.71
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.21	0.71
1:A:743:PRO:HG2	1:B:544:SER:HB3	1.73	0.71
1:C:777:TYR:C	1:C:780:LEU:HD11	2.11	0.71
2:D:65:PHE:HB2	2:D:66:PRO:HD3	1.73	0.71
2:D:7:GLU:HA	2:D:10:ALA:HB3	1.73	0.71
1:C:722:ILE:HD13	1:C:764:LEU:CD2	2.20	0.71
1:B:726:ILE:CA	1:B:729:TYR:HB2	2.19	0.70
1:C:667:LEU:O	1:C:671:ARG:HB2	1.89	0.70
1:C:734:ASN:HA	1:C:737:LYS:HB2	1.71	0.70
2:F:7:GLU:HA	2:F:10:ALA:HB3	1.73	0.70
1:B:526:GLN:H	1:B:526:GLN:HE21	1.36	0.70
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.73	0.70
2:E:7:GLU:HA	2:E:10:ALA:HB3	1.73	0.70
1:A:659:THR:CG2	1:A:662:GLU:H	2.05	0.70
1:B:366:PHE:HA	1:B:477:MET:CE	2.22	0.70
1:A:456:LYS:CB	1:A:470:ASN:O	2.40	0.70
2:F:138:TYR:O	2:F:142:VAL:HG23	1.92	0.70
1:A:510:GLN:O	1:A:510:GLN:HG3	1.91	0.70
1:A:777:TYR:O	1:A:780:LEU:HD11	1.92	0.70
1:C:304:ALA:HB3	1:C:604:LEU:HD13	1.74	0.70
1:A:324:THR:HG21	1:A:556:MET:HE1	1.74	0.69
1:C:463:THR:HG22	1:C:465:LEU:N	2.03	0.69
1:A:504:ILE:CD1	1:A:625:LEU:HD22	2.23	0.69
1:A:666:ASN:O	1:A:670:ILE:HB	1.92	0.69
1:A:736:LEU:HD21	1:A:749:PHE:HB2	1.73	0.69
1:B:478:ALA:HB1	1:B:486:LYS:O	1.91	0.69
1:C:747:ASN:O	1:C:750:GLN:HG2	1.91	0.69
1:A:776:LEU:H	1:A:776:LEU:HD12	1.56	0.69
1:B:785:ASN:OD1	1:B:787:THR:HG23	1.91	0.69
1:A:714:GLN:NE2	1:A:714:GLN:HA	2.06	0.69
1:C:736:LEU:HD21	1:C:749:PHE:HB2	1.75	0.69
2:E:65:PHE:HB2	2:E:66:PRO:HD3	1.73	0.69
2:F:65:PHE:HB2	2:F:66:PRO:HD3	1.72	0.69
1:B:324:THR:HG22	1:B:499:PRO:CA	2.21	0.68
1:C:785:ASN:OD1	1:C:786:GLU:HG2	1.93	0.68
2:D:13:LYS:HG3	2:D:65:PHE:CE2	2.28	0.68
1:B:513:TRP:CZ2	2:E:112:LEU:O	2.47	0.68
2:E:138:TYR:O	2:E:142:VAL:HG23	1.94	0.68
2:E:13:LYS:HG3	2:E:65:PHE:CE2	2.29	0.68
1:A:789:ASN:ND2	1:A:789:ASN:N	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:VAL:N	1:B:610:MET:HE1	2.08	0.68
1:B:535:LYS:HE2	1:B:535:LYS:CA	2.21	0.68
1:B:793:PHE:HA	1:B:796:ILE:CG1	2.23	0.68
1:C:639:ASN:ND2	1:C:641:ALA:H	1.90	0.68
1:B:722:ILE:HG23	1:B:760:VAL:HG11	1.76	0.68
1:B:375:GLY:O	1:B:376:GLN:HB2	1.94	0.67
1:A:509:PRO:HG2	1:A:512:GLU:HB2	1.77	0.67
1:A:747:ASN:O	1:A:750:GLN:HG2	1.94	0.67
1:B:424:LYS:HE2	1:B:433:TYR:OH	1.95	0.67
1:B:508:ILE:HG23	1:B:536:TYR:CD1	2.30	0.67
1:C:534:ILE:HA	1:C:538:ILE:HB	1.77	0.67
1:B:655:ASN:N	1:B:755:ARG:HD2	2.09	0.67
2:F:13:LYS:HG3	2:F:65:PHE:CE2	2.30	0.67
1:A:445:ARG:CZ	1:A:471:TRP:HE1	2.08	0.67
1:B:322:LEU:O	1:B:324:THR:HG23	1.95	0.66
1:B:720:ILE:O	1:B:724:ARG:HG2	1.95	0.66
1:B:714:GLN:HE22	1:B:715:GLU:HG3	1.59	0.66
1:B:537:GLY:O	1:B:625:LEU:HD21	1.95	0.66
1:B:727:GLN:HG3	1:B:786:GLU:CD	2.15	0.66
1:C:349:ASN:N	1:C:349:ASN:HD22	1.89	0.66
2:F:8:GLN:HE21	2:F:8:GLN:HA	1.61	0.66
1:B:654:ILE:HA	1:B:755:ARG:HD3	1.78	0.66
1:C:657:ILE:HG13	1:C:759:GLN:HG2	1.78	0.66
1:A:780:LEU:HD12	1:A:780:LEU:H	1.59	0.66
1:A:295:VAL:HG21	1:A:603:ILE:HG22	1.77	0.66
1:C:671:ARG:HD2	2:F:14:GLU:OE2	1.96	0.65
2:D:138:TYR:O	2:D:142:VAL:HG23	1.96	0.65
2:E:8:GLN:HE21	2:E:8:GLN:HA	1.60	0.65
1:B:792:VAL:O	1:B:796:ILE:HG12	1.96	0.65
1:C:777:TYR:O	1:C:780:LEU:HD11	1.97	0.65
2:D:8:GLN:HA	2:D:8:GLN:HE21	1.62	0.65
2:E:12:PHE:CD1	2:E:39:LEU:HD21	2.29	0.65
2:E:95:ASP:OD1	2:E:104:GLU:OE2	2.15	0.65
2:F:12:PHE:CD1	2:F:39:LEU:HD21	2.30	0.65
1:A:781:ASN:HB2	1:A:789:ASN:CG	2.17	0.65
2:D:83:GLU:O	2:D:87:GLU:HG3	1.96	0.65
1:C:659:THR:HG22	1:C:661:ALA:N	2.12	0.65
1:A:695:LYS:CD	2:D:19:PHE:HB2	2.27	0.65
1:B:551:ASN:HD22	1:B:551:ASN:N	1.88	0.65
1:B:335:ALA:HB1	1:B:489:THR:HG21	1.77	0.64
1:B:520:PRO:CB	1:B:524:GLU:OE1	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:THR:HA	1:B:773:PHE:CE1	2.33	0.64
2:D:12:PHE:CD1	2:D:39:LEU:HD21	2.30	0.64
1:C:780:LEU:HD12	1:C:780:LEU:H	1.63	0.64
1:A:714:GLN:OE1	2:D:126:ARG:HG3	1.97	0.64
1:B:514:ASP:HA	1:B:517:VAL:CG1	2.28	0.64
1:B:752:LEU:CD2	1:B:756:ILE:HD11	2.27	0.64
1:B:327:LEU:CD2	1:B:496:ALA:HB3	2.22	0.64
2:D:5:THR:OG1	2:D:8:GLN:HG2	1.97	0.64
1:B:450:ASN:O	1:B:451:ASN:HB2	1.95	0.64
1:A:629:ASN:HD22	1:A:631:SER:N	1.92	0.64
1:B:550:SER:H	1:B:553:GLN:NE2	1.95	0.64
1:B:764:LEU:HD22	1:B:768:LYS:HD3	1.79	0.64
1:C:504:ILE:CD1	1:C:625:LEU:HD22	2.28	0.64
1:B:297:LYS:HZ1	1:B:601:GLU:HB3	1.63	0.63
1:C:517:VAL:HG13	1:C:518:ASN:ND2	2.14	0.63
1:A:304:ALA:HB3	1:A:604:LEU:HD13	1.80	0.63
1:C:530:THR:HG21	2:F:145:MET:SD	2.38	0.63
1:B:462:ILE:HG23	1:B:467:GLU:O	1.99	0.63
1:B:726:ILE:HA	1:B:729:TYR:CB	2.20	0.63
1:A:445:ARG:HE	1:A:471:TRP:HE1	1.43	0.63
1:A:696:LYS:HD3	1:A:731:GLU:OE1	1.99	0.63
1:B:750:GLN:O	1:B:753:LYS:HB3	1.99	0.63
1:C:659:THR:HG22	1:C:661:ALA:H	1.62	0.63
2:F:36:MET:O	2:F:41:GLN:HB2	1.99	0.63
2:E:37:ARG:HA	2:E:41:GLN:O	1.98	0.62
1:B:369:ASP:OD2	1:B:442:TYR:OH	2.12	0.62
2:E:36:MET:O	2:E:41:GLN:HB2	1.99	0.62
2:F:37:ARG:HA	2:F:41:GLN:O	1.99	0.62
1:A:456:LYS:CD	1:A:471:TRP:HD1	2.11	0.62
1:A:706:ASN:HD21	1:A:708:ALA:HB3	1.64	0.62
1:B:551:ASN:O	1:B:555:GLN:HG3	2.00	0.62
2:F:75:LYS:O	2:F:79:THR:HG22	1.99	0.62
1:B:639:ASN:HD22	1:B:641:ALA:H	1.45	0.62
1:C:660:SER:O	1:C:663:PHE:HB3	1.99	0.62
1:C:706:ASN:HD21	1:C:708:ALA:HB3	1.64	0.62
2:D:37:ARG:HA	2:D:41:GLN:O	1.99	0.62
2:E:75:LYS:O	2:E:79:THR:HG22	1.99	0.62
1:A:513:TRP:O	1:A:517:VAL:HG23	1.99	0.62
1:A:648:PRO:HA	1:A:651:LYS:HD2	1.81	0.62
1:B:332:ASN:C	1:B:332:ASN:HD22	2.03	0.62
1:B:508:ILE:HG23	1:B:536:TYR:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:PHE:CD1	1:B:477:MET:HE1	2.32	0.62
1:C:508:ILE:HG23	1:C:536:TYR:CE2	2.35	0.62
1:C:295:VAL:HG23	1:C:604:LEU:O	2.00	0.61
1:C:730:ASN:O	1:C:733:GLU:HB2	2.00	0.61
1:B:298:GLY:O	1:B:299:GLU:C	2.38	0.61
1:C:327:LEU:N	1:C:327:LEU:HD12	2.14	0.61
1:C:380:VAL:HG12	1:C:384:ASN:ND2	2.14	0.61
1:A:463:THR:HB	1:A:467:GLU:H	1.63	0.61
1:B:312:ALA:O	1:B:315:PHE:HB2	2.01	0.61
1:B:738:SER:CB	1:B:741:ILE:HD11	2.28	0.61
1:B:784:GLU:HG2	1:B:788:ASP:OD2	1.99	0.61
1:C:535:LYS:HD2	1:C:536:TYR:CZ	2.35	0.61
2:D:75:LYS:O	2:D:79:THR:HG22	2.00	0.61
1:A:323:ASN:HD22	1:A:598:PRO:HB3	1.66	0.61
1:A:743:PRO:HG2	1:B:544:SER:CB	2.30	0.61
1:B:492:TYR:CD2	1:B:574:VAL:HG13	2.36	0.61
1:B:605:THR:CG2	1:B:611:THR:OG1	2.45	0.61
1:A:538:ILE:HG22	1:A:539:GLU:N	2.16	0.61
1:B:297:LYS:NZ	1:B:601:GLU:HB3	2.16	0.61
1:B:734:ASN:C	1:B:736:LEU:H	2.04	0.61
1:A:462:ILE:HG13	1:A:466:GLY:HA2	1.83	0.61
1:B:788:ASP:O	1:B:791:GLU:HG2	2.00	0.61
1:C:668:SER:CB	2:F:14:GLU:HG3	2.30	0.61
1:B:657:ILE:HG12	1:B:658:PRO:HD2	1.83	0.61
1:B:706:ASN:HB2	1:B:724:ARG:HH22	1.66	0.61
1:B:744:GLU:OE1	1:B:744:GLU:HA	1.99	0.61
1:B:722:ILE:HG23	1:B:760:VAL:CG1	2.31	0.61
1:B:525:LYS:O	1:B:527:LYS:N	2.34	0.60
1:B:729:TYR:HE2	1:B:773:PHE:CE1	2.19	0.60
1:B:792:VAL:HG12	1:B:796:ILE:HD11	1.82	0.60
1:C:657:ILE:HG13	1:C:759:GLN:CG	2.31	0.60
1:B:542:PRO:HA	1:B:548:THR:HA	1.82	0.60
1:B:706:ASN:CB	1:B:724:ARG:HH22	2.13	0.60
1:A:380:VAL:HG12	1:A:384:ASN:HD21	1.65	0.60
1:A:784:GLU:OE1	1:A:785:ASN:ND2	2.34	0.60
1:B:332:ASN:HD22	1:B:334:LEU:H	1.50	0.60
1:B:298:GLY:O	1:B:300:LYS:N	2.35	0.60
1:B:622:LYS:O	1:B:623:ASP:HB2	2.02	0.60
1:B:714:GLN:O	1:B:718:ARG:HG3	2.01	0.60
1:B:751:TYR:HA	1:B:754:GLU:OE2	2.01	0.60
1:C:324:THR:HG21	1:C:556:MET:CE	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:PHE:CD2	2:E:108:VAL:HG21	2.37	0.60
2:F:65:PHE:O	2:F:69:LEU:HG	2.01	0.60
1:B:761:GLN:HG3	1:B:765:THR:CG2	2.31	0.60
1:C:792:VAL:O	1:C:796:ILE:HG12	2.02	0.60
1:B:360:VAL:CG2	1:B:365:PRO:HG3	2.27	0.60
1:B:597:ASN:ND2	1:B:601:GLU:HB2	2.16	0.60
1:C:558:ASP:O	1:C:562:GLU:HG3	2.01	0.60
1:C:581:GLN:HE21	1:C:628:PHE:HA	1.66	0.60
1:A:517:VAL:HG13	2:D:114:GLU:OE2	2.02	0.60
1:A:512:GLU:O	1:A:516:VAL:HG23	2.02	0.60
1:A:697:ILE:HD13	1:A:732:ILE:CG1	2.32	0.60
2:D:115:LYS:HB3	2:D:115:LYS:HZ2	1.67	0.60
1:C:784:GLU:CD	1:C:784:GLU:N	2.55	0.59
1:A:605:THR:HG21	1:A:611:THR:HA	1.84	0.59
1:A:797:ILE:HG13	1:A:798:ASP:N	2.16	0.59
1:C:797:ILE:HG13	1:C:798:ASP:N	2.16	0.59
1:A:654:ILE:HG23	1:A:655:ASN:ND2	2.16	0.59
1:C:792:VAL:HG12	1:C:796:ILE:HD11	1.84	0.59
1:B:561:ASN:O	1:B:564:VAL:HG22	2.03	0.59
1:B:761:GLN:HG3	1:B:765:THR:HG23	1.84	0.59
2:E:8:GLN:NE2	2:E:8:GLN:HA	2.17	0.59
2:F:115:LYS:HB3	2:F:115:LYS:HZ2	1.67	0.59
1:A:380:VAL:HG12	1:A:384:ASN:ND2	2.17	0.59
1:A:792:VAL:HG12	1:A:796:ILE:HD11	1.84	0.59
1:C:510:GLN:HG3	1:C:510:GLN:O	2.02	0.59
1:C:651:LYS:O	1:C:654:ILE:HG13	2.02	0.59
1:A:491:ASP:OD2	1:A:491:ASP:C	2.41	0.59
1:A:730:ASN:O	1:A:733:GLU:HB2	2.03	0.59
1:B:305:SER:HB2	1:B:307:LEU:HD13	1.85	0.59
1:B:564:VAL:O	1:B:567:THR:HB	2.02	0.59
1:B:294:ASP:C	1:B:610:MET:HE1	2.22	0.59
1:B:329:ARG:NH1	1:B:590:ASP:OD2	2.34	0.59
1:C:657:ILE:HG12	1:C:756:ILE:HA	1.82	0.59
1:A:408:LEU:O	1:A:412:GLU:HG3	2.03	0.59
1:B:366:PHE:HD1	1:B:477:MET:HE2	1.67	0.59
1:A:377:GLN:HB2	1:A:464:VAL:HG12	1.85	0.58
1:A:792:VAL:O	1:A:796:ILE:HG12	2.03	0.58
1:B:459:GLU:O	1:B:461:LYS:N	2.36	0.58
1:B:519:THR:OG1	1:B:521:ASN:ND2	2.36	0.58
1:A:540:ARG:HD3	1:A:627:TYR:OH	2.03	0.58
1:B:751:TYR:HA	1:B:754:GLU:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:PHE:O	2:D:69:LEU:HG	2.03	0.58
1:B:619:ILE:C	1:B:621:GLY:H	2.06	0.58
1:C:324:THR:HG21	1:C:556:MET:HE1	1.86	0.58
1:A:504:ILE:HD11	1:A:625:LEU:HD22	1.84	0.58
1:B:489:THR:HG22	1:B:490:ALA:N	2.11	0.58
2:F:95:ASP:OD1	2:F:104:GLU:OE2	2.21	0.58
1:B:508:ILE:HG21	1:B:532:LEU:HD22	1.85	0.58
1:B:615:ILE:HD12	1:B:645:TRP:CH2	2.39	0.58
1:C:549:LEU:N	1:C:549:LEU:HD12	2.19	0.58
1:C:629:ASN:ND2	1:C:631:SER:HB2	2.19	0.58
1:C:623:ASP:OD1	2:F:94:LYS:HD3	2.04	0.58
1:A:785:ASN:O	1:A:786:GLU:CG	2.52	0.58
1:B:723:PHE:HB2	1:B:793:PHE:CE2	2.39	0.58
1:C:540:ARG:NH1	1:C:627:TYR:CE1	2.72	0.58
2:D:36:MET:O	2:D:41:GLN:HB2	2.04	0.58
1:C:766:HIS:NE2	2:F:133:ASP:O	2.36	0.58
1:A:581:GLN:HE21	1:A:628:PHE:HA	1.68	0.58
2:E:115:LYS:HB3	2:E:115:LYS:HZ2	1.69	0.58
1:B:613:ARG:O	1:B:616:GLU:HG2	2.04	0.58
2:F:8:GLN:NE2	2:F:8:GLN:HA	2.19	0.58
1:B:605:THR:HG21	1:B:611:THR:HG1	1.69	0.57
1:B:722:ILE:HD13	1:B:764:LEU:HD21	1.85	0.57
1:A:432:TYR:CE1	1:A:471:TRP:HZ3	2.23	0.57
1:B:366:PHE:CD1	1:B:477:MET:CE	2.82	0.57
1:B:551:ASN:ND2	1:B:551:ASN:N	2.39	0.57
1:B:639:ASN:O	1:B:640:LYS:HB2	2.03	0.57
1:C:406:ASP:OD1	1:C:408:LEU:N	2.38	0.57
1:C:731:GLU:O	1:C:735:VAL:HG23	2.03	0.57
1:A:785:ASN:O	1:A:786:GLU:HG2	2.03	0.57
1:A:445:ARG:NH2	1:A:471:TRP:HE1	2.02	0.57
1:A:719:LYS:HE2	1:A:797:ILE:HD13	1.84	0.57
1:A:731:GLU:O	1:A:735:VAL:HG23	2.05	0.57
1:B:719:LYS:HD2	1:B:794:GLN:HG3	1.87	0.57
1:B:323:ASN:OD1	1:B:500:SER:HB3	2.04	0.57
1:C:629:ASN:HB3	1:C:632:TYR:CD2	2.39	0.57
1:A:505:LYS:HD3	2:D:112:LEU:O	2.05	0.57
1:B:426:ILE:HA	1:B:430:LYS:O	2.04	0.57
1:C:505:LYS:HE3	1:C:513:TRP:CD2	2.39	0.57
1:C:666:ASN:HD22	1:C:666:ASN:N	2.00	0.57
1:A:789:ASN:HD22	1:A:789:ASN:H	1.50	0.57
1:B:597:ASN:HD21	1:B:601:GLU:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLN:HA	2:D:8:GLN:NE2	2.20	0.57
2:D:144:MET:SD	2:D:145:MET:HE2	2.44	0.57
1:A:540:ARG:HD3	1:A:627:TYR:CZ	2.40	0.56
1:B:394:HIS:O	1:B:397:GLU:HG2	2.05	0.56
1:B:335:ALA:HB1	1:B:489:THR:HG22	1.86	0.56
1:C:789:ASN:H	1:C:789:ASN:HD22	1.50	0.56
2:E:63:ILE:HD12	2:E:63:ILE:N	2.20	0.56
2:F:25:GLY:O	2:F:64:ASP:HA	2.04	0.56
2:F:63:ILE:N	2:F:63:ILE:HD12	2.20	0.56
1:B:506:LYS:HG2	1:B:506:LYS:O	2.05	0.56
1:B:746:LYS:O	1:B:750:GLN:HB2	2.05	0.56
1:C:633:ASN:ND2	1:C:645:TRP:H	1.98	0.56
1:C:776:LEU:H	1:C:776:LEU:CD1	2.18	0.56
2:E:65:PHE:O	2:E:69:LEU:HG	2.05	0.56
1:A:327:LEU:HD12	1:A:327:LEU:N	2.20	0.56
1:A:549:LEU:HD12	1:A:549:LEU:N	2.21	0.56
1:C:456:LYS:HD3	1:C:471:TRP:CD2	2.41	0.56
1:C:633:ASN:ND2	1:C:644:GLU:HA	2.21	0.56
1:C:753:LYS:NZ	1:C:753:LYS:HB3	2.21	0.56
1:B:375:GLY:HA2	1:B:464:VAL:HG11	1.88	0.56
1:B:549:LEU:HD21	1:B:554:LYS:HG2	1.88	0.55
1:B:513:TRP:CH2	2:E:113:GLY:HA3	2.41	0.55
2:E:27:ILE:HB	2:E:31:GLU:HG3	1.86	0.55
1:A:695:LYS:HD3	2:D:19:PHE:HB2	1.87	0.55
1:A:697:ILE:HD13	1:A:732:ILE:HG12	1.88	0.55
1:B:727:GLN:HG3	1:B:786:GLU:OE1	2.06	0.55
1:C:510:GLN:NE2	1:C:510:GLN:HA	2.20	0.55
1:B:516:VAL:HA	1:B:520:PRO:HG2	1.88	0.55
1:B:540:ARG:HD2	1:B:627:TYR:CZ	2.41	0.55
2:D:27:ILE:HB	2:D:31:GLU:HG3	1.87	0.55
1:A:630:ARG:HD3	2:D:83:GLU:OE2	2.07	0.55
2:E:70:THR:O	2:E:73:ALA:HB3	2.07	0.55
2:E:144:MET:SD	2:E:145:MET:HE2	2.47	0.55
1:B:550:SER:O	1:B:553:GLN:HB2	2.07	0.55
1:C:318:ILE:N	1:C:318:ILE:HD12	2.21	0.55
1:C:540:ARG:HD2	1:C:582:ASP:OD1	2.06	0.55
1:C:605:THR:HG21	1:C:611:THR:HA	1.89	0.55
1:B:773:PHE:C	1:B:775:LEU:N	2.56	0.55
2:D:19:PHE:C	2:D:19:PHE:CD1	2.80	0.55
1:C:462:ILE:HG13	1:C:466:GLY:HA2	1.88	0.55
2:F:27:ILE:HB	2:F:31:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:OD1	1:A:408:LEU:N	2.40	0.55
1:C:491:ASP:C	1:C:491:ASP:OD2	2.45	0.55
1:C:698:ALA:O	1:C:701:LEU:HB2	2.06	0.55
2:D:25:GLY:O	2:D:64:ASP:HA	2.07	0.55
2:E:133:ASP:OD2	2:E:135:GLN:HG3	2.07	0.55
1:A:377:GLN:HB2	1:A:464:VAL:CG1	2.37	0.55
1:B:549:LEU:CD2	1:B:554:LYS:HG2	2.37	0.55
2:D:63:ILE:N	2:D:63:ILE:HD12	2.21	0.55
1:A:697:ILE:HD11	1:A:732:ILE:N	2.22	0.54
1:B:639:ASN:HD22	1:B:640:LYS:N	2.05	0.54
1:C:668:SER:HA	2:F:14:GLU:HG3	1.90	0.54
1:C:661:ALA:C	1:C:663:PHE:H	2.10	0.54
2:D:55:VAL:HG13	2:D:56:ASP:N	2.22	0.54
1:B:655:ASN:H	1:B:755:ARG:HD2	1.71	0.54
1:C:655:ASN:HA	1:C:758:ASN:HB2	1.89	0.54
1:C:789:ASN:ND2	1:C:789:ASN:N	2.40	0.54
2:D:70:THR:O	2:D:73:ALA:HB3	2.08	0.54
1:A:318:ILE:HD12	1:A:318:ILE:N	2.22	0.54
1:C:408:LEU:O	1:C:412:GLU:HG3	2.08	0.54
1:B:514:ASP:CA	1:B:517:VAL:HG12	2.35	0.54
1:C:549:LEU:H	1:C:549:LEU:HD12	1.73	0.54
1:A:629:ASN:ND2	1:A:631:SER:HB2	2.22	0.54
1:B:619:ILE:C	1:B:621:GLY:N	2.60	0.54
1:B:716:LYS:O	1:B:719:LYS:HB3	2.08	0.54
1:C:787:THR:O	1:C:787:THR:HG22	2.07	0.54
1:B:596:ILE:HA	1:B:601:GLU:O	2.07	0.54
1:C:318:ILE:HD12	1:C:318:ILE:H	1.72	0.54
1:B:513:TRP:HH2	2:E:113:GLY:HA3	1.73	0.54
1:A:438:ASN:HD22	1:A:438:ASN:C	2.11	0.54
1:A:540:ARG:NH1	1:A:627:TYR:CE1	2.75	0.54
1:A:700:TYR:CE1	1:A:727:GLN:HB3	2.43	0.54
1:A:657:ILE:HD11	1:A:704:TYR:CG	2.42	0.54
1:B:780:LEU:HB3	1:B:782:PHE:CE1	2.43	0.54
1:B:793:PHE:CA	1:B:796:ILE:HG12	2.32	0.54
1:C:320:ARG:HG3	1:C:598:PRO:O	2.07	0.54
2:E:102:ALA:HB2	2:E:125:ILE:HG13	1.90	0.54
1:B:748:TYR:HD2	1:B:749:PHE:CD2	2.26	0.53
1:C:510:GLN:O	1:C:514:ASP:OD1	2.25	0.53
1:C:540:ARG:HD3	1:C:627:TYR:OH	2.09	0.53
2:F:44:THR:OG1	2:F:47:GLU:HG3	2.08	0.53
1:B:294:ASP:O	1:B:606:LYS:HE3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:ILE:HD13	1:C:537:GLY:HA3	1.89	0.53
1:C:623:ASP:H	2:F:94:LYS:HD2	1.72	0.53
1:A:670:ILE:O	1:A:670:ILE:HD13	2.08	0.53
2:D:133:ASP:OD2	2:D:135:GLN:HG3	2.08	0.53
2:E:25:GLY:O	2:E:64:ASP:HA	2.07	0.53
1:B:650:THR:HA	1:B:653:LYS:HB2	1.91	0.53
1:B:714:GLN:NE2	1:B:715:GLU:HG3	2.23	0.53
1:C:535:LYS:HD2	1:C:536:TYR:CE1	2.44	0.53
1:C:758:ASN:O	1:C:762:LEU:HB2	2.09	0.53
2:E:105:LEU:HD12	2:E:125:ILE:CD1	2.39	0.53
2:E:44:THR:OG1	2:E:47:GLU:HG3	2.09	0.53
1:B:550:SER:N	1:B:553:GLN:NE2	2.56	0.53
1:B:756:ILE:O	1:B:760:VAL:HG23	2.08	0.53
1:C:712:PHE:HB3	1:C:716:LYS:HG2	1.89	0.53
1:A:334:LEU:HD13	1:A:361:ALA:HB1	1.90	0.53
1:B:299:GLU:HB3	1:B:303:LYS:HZ3	1.74	0.53
1:C:510:GLN:HE21	1:C:510:GLN:HA	1.74	0.53
1:C:377:GLN:HB2	1:C:464:VAL:HG12	1.91	0.53
1:B:552:TRP:C	1:B:552:TRP:CD1	2.82	0.53
2:D:101:SER:OG	2:D:104:GLU:HG3	2.08	0.53
1:C:505:LYS:HD3	2:F:112:LEU:O	2.09	0.53
1:B:508:ILE:HG22	1:B:509:PRO:HD2	1.90	0.52
1:B:776:LEU:HB3	1:B:779:GLN:HG3	1.90	0.52
1:C:629:ASN:HB3	1:C:632:TYR:CE2	2.44	0.52
2:F:70:THR:O	2:F:73:ALA:HB3	2.09	0.52
1:A:463:THR:CG2	1:A:464:VAL:N	2.72	0.52
1:B:773:PHE:C	1:B:775:LEU:H	2.13	0.52
1:C:550:SER:H	1:C:553:GLN:NE2	2.06	0.52
1:C:723:PHE:HB2	1:C:793:PHE:CE2	2.45	0.52
2:F:133:ASP:OD2	2:F:135:GLN:HG3	2.09	0.52
2:F:55:VAL:HG13	2:F:56:ASP:N	2.24	0.52
1:A:595:ILE:HB	1:A:603:ILE:HB	1.92	0.52
1:B:305:SER:HB3	1:B:594:PHE:CD1	2.44	0.52
1:B:332:ASN:HD22	1:B:333:LYS:N	2.06	0.52
1:C:639:ASN:C	1:C:639:ASN:HD22	2.13	0.52
1:C:691:LYS:O	1:C:694:VAL:HG13	2.09	0.52
1:A:776:LEU:H	1:A:776:LEU:CD1	2.22	0.52
1:C:295:VAL:HG22	1:C:296:LEU:O	2.08	0.52
1:C:559:ARG:O	1:C:562:GLU:HB2	2.09	0.52
1:C:595:ILE:HB	1:C:603:ILE:HB	1.92	0.52
1:A:550:SER:O	1:A:554:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ASN:C	1:A:639:ASN:HD22	2.12	0.52
1:A:695:LYS:HA	2:D:18:LEU:HD22	1.92	0.52
1:A:787:THR:HG22	1:A:791:GLU:OE2	2.09	0.52
1:B:456:LYS:HB3	1:B:470:ASN:O	2.09	0.52
1:B:540:ARG:CZ	1:B:627:TYR:CE1	2.93	0.52
1:B:706:ASN:O	1:B:709:ASN:HB2	2.10	0.52
1:B:712:PHE:HD1	1:B:712:PHE:H	1.57	0.52
1:C:742:ALA:HB3	1:C:745:TYR:CB	2.38	0.52
2:F:19:PHE:CD1	2:F:19:PHE:C	2.82	0.52
1:C:514:ASP:N	1:C:514:ASP:OD2	2.41	0.52
2:F:92:PHE:CD2	2:F:108:VAL:HG21	2.44	0.52
1:A:780:LEU:HD12	1:A:780:LEU:N	2.25	0.52
1:B:587:PRO:HB2	1:B:643:ILE:HD12	1.92	0.52
1:C:463:THR:CG2	1:C:464:VAL:N	2.72	0.52
1:B:504:ILE:HG23	1:B:536:TYR:O	2.09	0.52
1:C:597:ASN:HB2	1:C:598:PRO:HD2	1.92	0.52
1:C:668:SER:CA	2:F:14:GLU:HG3	2.39	0.52
1:C:786:GLU:O	1:C:788:ASP:N	2.39	0.52
1:A:295:VAL:HG22	1:A:296:LEU:O	2.10	0.52
1:A:785:ASN:C	1:A:786:GLU:HG2	2.30	0.52
1:B:707:SER:O	1:B:709:ASN:N	2.42	0.52
1:B:718:ARG:O	1:B:722:ILE:HG13	2.10	0.52
1:A:523:LEU:CD1	2:D:127:GLU:HB3	2.40	0.52
2:E:55:VAL:HG13	2:E:56:ASP:N	2.25	0.52
1:C:550:SER:O	1:C:554:LYS:HG3	2.10	0.51
1:B:373:LYS:O	1:B:375:GLY:O	2.28	0.51
1:B:464:VAL:C	1:B:466:GLY:H	2.14	0.51
2:E:97:ASN:HD21	2:E:99:TYR:HB2	1.75	0.51
1:A:753:LYS:HB3	1:A:753:LYS:NZ	2.26	0.51
1:A:787:THR:HG22	1:A:791:GLU:CD	2.31	0.51
1:C:295:VAL:HG21	1:C:603:ILE:HG23	1.87	0.51
1:C:377:GLN:HB2	1:C:464:VAL:CG1	2.40	0.51
1:A:695:LYS:HD2	2:D:18:LEU:HB3	1.93	0.51
1:A:697:ILE:HG12	1:A:731:GLU:HB2	1.93	0.51
1:B:626:TYR:CD2	1:B:627:TYR:N	2.79	0.51
1:C:313:ASP:HA	1:C:316:LYS:HE2	1.93	0.51
2:D:44:THR:OG1	2:D:47:GLU:HG3	2.09	0.51
1:A:349:ASN:N	1:A:349:ASN:ND2	2.56	0.51
1:A:672:ARG:O	1:A:674:SER:N	2.39	0.51
1:B:616:GLU:HA	1:B:620:THR:CG2	2.21	0.51
1:C:501:LEU:H	1:C:501:LEU:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:GLU:O	2:D:114:GLU:HG3	2.10	0.51
1:B:492:TYR:HD2	1:B:574:VAL:HG13	1.75	0.51
1:B:615:ILE:HD12	1:B:645:TRP:CZ2	2.46	0.51
1:C:540:ARG:HD3	1:C:627:TYR:CZ	2.46	0.51
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.93	0.51
1:C:791:GLU:OE1	1:C:791:GLU:N	2.44	0.51
2:E:116:LEU:HD22	2:E:120:GLU:OE2	2.11	0.51
1:A:629:ASN:HB3	1:A:632:TYR:CD2	2.46	0.51
1:B:320:ARG:CG	1:B:321:GLU:H	2.22	0.51
1:B:761:GLN:O	1:B:765:THR:N	2.29	0.51
2:F:29:THR:OG1	2:F:52:ILE:HG12	2.11	0.51
1:A:723:PHE:HB2	1:A:793:PHE:CE2	2.46	0.51
1:B:316:LYS:HG2	1:B:600:GLY:O	2.10	0.51
1:B:550:SER:N	1:B:553:GLN:HE21	2.04	0.51
1:B:657:ILE:CG1	1:B:658:PRO:HD2	2.41	0.51
2:D:133:ASP:N	2:D:133:ASP:OD1	2.30	0.51
1:A:540:ARG:NH1	1:A:582:ASP:OD1	2.42	0.51
1:A:742:ALA:HB3	1:A:745:TYR:CB	2.37	0.51
1:C:320:ARG:HA	1:C:598:PRO:O	2.11	0.51
1:C:776:LEU:HD12	1:C:776:LEU:N	2.21	0.51
1:A:540:ARG:NH2	2:D:87:GLU:OE1	2.44	0.51
2:F:105:LEU:HD12	2:F:125:ILE:CD1	2.40	0.51
1:A:712:PHE:HB3	1:A:716:LYS:HG2	1.92	0.50
1:B:500:SER:HA	1:B:624:TYR:CD2	2.46	0.50
1:A:787:THR:C	1:A:791:GLU:OE1	2.49	0.50
1:B:505:LYS:C	1:B:507:GLN:H	2.14	0.50
1:B:602:PHE:C	1:B:603:ILE:HG13	2.32	0.50
2:D:102:ALA:HB2	2:D:125:ILE:HG13	1.91	0.50
2:D:116:LEU:HD22	2:D:120:GLU:OE2	2.11	0.50
2:F:116:LEU:HD22	2:F:120:GLU:OE2	2.11	0.50
1:B:320:ARG:CG	1:B:321:GLU:N	2.73	0.50
1:C:508:ILE:HG21	1:C:532:LEU:HD13	1.93	0.50
1:A:492:TYR:HD2	1:A:574:VAL:HG13	1.77	0.50
1:B:318:ILE:N	1:B:318:ILE:HD12	2.26	0.50
1:B:733:GLU:C	1:B:735:VAL:H	2.15	0.50
1:C:657:ILE:HG23	1:C:756:ILE:CD1	2.41	0.50
2:E:29:THR:OG1	2:E:52:ILE:HG12	2.11	0.50
1:B:623:ASP:OD1	2:E:94:LYS:HD3	2.11	0.50
1:A:550:SER:H	1:A:553:GLN:NE2	2.09	0.50
1:B:384:ASN:O	1:B:388:LYS:HG3	2.11	0.50
1:C:663:PHE:HA	1:C:748:TYR:OH	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:ASP:N	2:E:133:ASP:OD1	2.35	0.50
2:E:80:ASP:C	2:E:82:GLU:H	2.14	0.50
2:F:68:PHE:O	2:F:72:MET:HG2	2.11	0.50
1:A:510:GLN:CG	1:A:510:GLN:O	2.58	0.50
1:B:318:ILE:HG23	1:B:322:LEU:HD12	1.94	0.50
1:C:349:ASN:ND2	1:C:349:ASN:H	1.99	0.50
1:C:657:ILE:CG1	1:C:759:GLN:HG2	2.40	0.50
1:A:540:ARG:HD2	1:A:582:ASP:OD1	2.12	0.50
1:A:445:ARG:CZ	1:A:471:TRP:NE1	2.75	0.50
1:A:492:TYR:CD2	1:A:574:VAL:HG13	2.47	0.50
1:B:320:ARG:O	1:B:321:GLU:C	2.50	0.50
1:B:519:THR:HA	1:B:525:LYS:HE3	1.93	0.50
1:B:565:LYS:C	1:B:567:THR:H	2.14	0.50
1:A:758:ASN:O	1:A:762:LEU:HB2	2.11	0.49
1:B:403:LEU:HD13	1:B:476:VAL:HG21	1.94	0.49
1:C:705:TYR:CE2	2:F:139:GLU:HB3	2.47	0.49
1:B:565:LYS:O	1:B:567:THR:N	2.45	0.49
2:D:80:ASP:C	2:D:82:GLU:H	2.15	0.49
1:A:776:LEU:HD12	1:A:776:LEU:N	2.25	0.49
1:B:518:ASN:O	1:B:519:THR:CG2	2.59	0.49
1:C:401:ILE:HD13	1:C:478:ALA:HB2	1.94	0.49
2:D:29:THR:OG1	2:D:52:ILE:HG12	2.11	0.49
1:C:340:LYS:C	1:C:342:GLY:H	2.15	0.49
1:C:505:LYS:C	1:C:507:GLN:H	2.16	0.49
1:C:520:PRO:HG2	1:C:521:ASN:H	1.77	0.49
2:E:114:GLU:HG3	2:E:114:GLU:O	2.13	0.49
1:C:334:LEU:HD13	1:C:361:ALA:HB1	1.93	0.49
1:C:621:GLY:O	1:C:622:LYS:HD2	2.13	0.49
2:F:101:SER:OG	2:F:104:GLU:HG3	2.12	0.49
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.94	0.49
1:A:607:ASN:HD21	1:A:609:GLU:HB2	1.76	0.49
2:D:68:PHE:O	2:D:72:MET:HG2	2.12	0.49
2:E:10:ALA:O	2:E:14:GLU:HB2	2.13	0.49
2:F:97:ASN:HD21	2:F:99:TYR:HB2	1.77	0.49
1:B:333:LYS:O	1:B:336:THR:HG22	2.13	0.49
1:B:730:ASN:ND2	1:B:734:ASN:H	2.11	0.49
1:C:531:ASN:O	1:C:535:LYS:HB2	2.13	0.49
1:C:657:ILE:HG23	1:C:756:ILE:HD13	1.94	0.49
1:A:447:SER:O	1:A:451:ASN:HA	2.12	0.49
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.93	0.49
1:B:791:GLU:HG3	1:B:792:VAL:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ASP:OD2	1:C:442:TYR:OH	2.22	0.49
1:A:434:LEU:HD11	1:A:445:ARG:NH1	2.28	0.49
1:B:712:PHE:CD1	1:B:712:PHE:N	2.81	0.49
1:B:712:PHE:O	1:B:713:SER:O	2.31	0.49
1:C:316:LYS:HG2	1:C:600:GLY:O	2.12	0.49
2:E:102:ALA:HB1	2:E:121:VAL:HG12	1.94	0.49
1:A:657:ILE:HG22	1:A:756:ILE:HA	1.94	0.49
1:A:791:GLU:OE1	1:A:791:GLU:N	2.46	0.49
2:E:51:MET:C	2:E:53:ASN:H	2.16	0.49
1:A:607:ASN:O	1:A:610:MET:N	2.46	0.48
1:C:549:LEU:HD13	1:C:554:LYS:HE2	1.95	0.48
1:B:655:ASN:HB3	1:B:759:GLN:NE2	2.28	0.48
1:C:617:LYS:O	1:C:617:LYS:HD2	2.13	0.48
1:B:318:ILE:H	1:B:318:ILE:HD12	1.77	0.48
1:B:320:ARG:O	1:B:322:LEU:N	2.45	0.48
1:C:437:SER:C	1:C:439:ASN:H	2.16	0.48
1:C:656:THR:HG21	2:F:139:GLU:OE1	2.13	0.48
2:F:26:THR:HG22	2:F:64:ASP:HB3	1.95	0.48
2:F:52:ILE:O	2:F:52:ILE:HG13	2.13	0.48
1:A:659:THR:HG23	1:A:662:GLU:H	1.79	0.48
1:B:619:ILE:O	1:B:621:GLY:N	2.47	0.48
1:C:791:GLU:CD	1:C:791:GLU:N	2.67	0.48
1:A:639:ASN:HD22	1:A:641:ALA:H	1.61	0.48
1:B:360:VAL:O	1:B:360:VAL:CG2	2.62	0.48
1:B:654:ILE:O	1:B:655:ASN:ND2	2.46	0.48
2:F:97:ASN:ND2	2:F:99:TYR:HB2	2.29	0.48
1:A:340:LYS:C	1:A:342:GLY:H	2.16	0.48
1:B:649:ILE:O	1:B:649:ILE:HG22	2.13	0.48
1:C:509:PRO:O	1:C:511:LYS:N	2.42	0.48
1:B:313:ASP:O	1:B:315:PHE:N	2.46	0.48
1:B:450:ASN:OD1	1:B:452:GLU:HG3	2.14	0.48
1:B:580:GLU:OE1	1:B:587:PRO:HA	2.13	0.48
1:A:697:ILE:HD13	1:A:732:ILE:HG13	1.96	0.48
1:B:459:GLU:C	1:B:461:LYS:H	2.16	0.48
1:B:502:THR:O	1:B:505:LYS:HB3	2.14	0.48
1:B:605:THR:HG21	1:B:611:THR:CB	2.41	0.48
2:E:101:SER:OG	2:E:104:GLU:HG3	2.13	0.48
1:A:534:ILE:HA	1:A:538:ILE:HB	1.95	0.48
1:B:654:ILE:HA	1:B:755:ARG:CG	2.43	0.48
1:B:725:GLY:O	1:B:729:TYR:N	2.47	0.48
1:B:744:GLU:CD	1:C:397:GLU:HB2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:780:LEU:HD12	1:C:780:LEU:N	2.28	0.48
2:E:52:ILE:HG13	2:E:52:ILE:O	2.14	0.48
1:A:509:PRO:HG2	1:A:512:GLU:CB	2.42	0.48
1:B:335:ALA:O	1:B:339:ILE:HG13	2.14	0.48
1:B:348:LEU:HD12	1:B:545:THR:O	2.14	0.48
1:C:519:THR:OG1	1:C:520:PRO:CD	2.50	0.48
1:C:657:ILE:HG13	1:C:759:GLN:HB2	1.94	0.48
1:C:712:PHE:HB3	1:C:716:LYS:HB3	1.96	0.48
2:E:143:GLN:OE1	2:E:143:GLN:HA	2.14	0.48
2:F:144:MET:SD	2:F:145:MET:HE2	2.54	0.48
1:A:320:ARG:HA	1:A:598:PRO:O	2.13	0.47
1:A:316:LYS:HG2	1:A:600:GLY:O	2.14	0.47
1:B:489:THR:CG2	1:B:490:ALA:H	2.05	0.47
1:B:639:ASN:C	1:B:639:ASN:HD22	2.17	0.47
1:C:415:GLU:O	1:C:417:GLY:N	2.47	0.47
1:C:438:ASN:C	1:C:438:ASN:HD22	2.15	0.47
2:D:92:PHE:CD2	2:D:108:VAL:HG21	2.49	0.47
2:F:80:ASP:C	2:F:82:GLU:H	2.17	0.47
1:A:293:ILE:HG13	1:A:293:ILE:O	2.13	0.47
1:A:481:VAL:O	1:A:484:VAL:HG23	2.14	0.47
1:A:501:LEU:HD22	1:A:501:LEU:H	1.78	0.47
1:B:295:VAL:HG13	1:B:610:MET:HE1	1.95	0.47
1:A:630:ARG:CZ	2:D:83:GLU:HB3	2.44	0.47
1:A:718:ARG:O	1:A:722:ILE:HG13	2.15	0.47
1:B:540:ARG:HD2	1:B:627:TYR:OH	2.13	0.47
1:C:783:THR:HB	1:C:784:GLU:CD	2.33	0.47
2:F:133:ASP:OD1	2:F:133:ASP:N	2.33	0.47
2:F:51:MET:C	2:F:53:ASN:H	2.16	0.47
1:A:418:ILE:HG22	1:A:419:ILE:HG23	1.94	0.47
1:A:733:GLU:O	1:A:737:LYS:HE2	2.14	0.47
1:C:318:ILE:CD1	1:C:318:ILE:H	2.27	0.47
1:C:323:ASN:HD22	1:C:598:PRO:HB3	1.80	0.47
1:C:328:PHE:O	1:C:593:ILE:HG23	2.14	0.47
1:C:505:LYS:HE3	1:C:513:TRP:CE2	2.50	0.47
2:D:8:GLN:CA	2:D:8:GLN:HE21	2.22	0.47
2:E:26:THR:HG22	2:E:64:ASP:HB3	1.95	0.47
2:E:68:PHE:O	2:E:72:MET:HG2	2.15	0.47
1:A:549:LEU:H	1:A:549:LEU:HD12	1.79	0.47
1:A:740:GLN:O	1:A:741:ILE:C	2.53	0.47
1:B:375:GLY:O	1:B:376:GLN:CB	2.58	0.47
1:B:570:THR:O	1:B:572:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:LEU:O	1:B:755:ARG:HB2	2.14	0.47
1:B:786:GLU:O	1:B:790:PHE:HB2	2.15	0.47
1:C:407:HIS:CD2	1:C:407:HIS:H	2.27	0.47
1:C:447:SER:O	1:C:451:ASN:HA	2.14	0.47
2:D:51:MET:C	2:D:53:ASN:H	2.17	0.47
1:A:633:ASN:ND2	1:A:644:GLU:HA	2.30	0.47
1:A:672:ARG:HG2	1:A:672:ARG:NH1	2.29	0.47
1:A:712:PHE:HB3	1:A:716:LYS:HB3	1.95	0.47
2:D:146:THR:OG1	2:D:147:ALA:N	2.47	0.47
2:D:76:MET:HA	2:D:79:THR:CG2	2.44	0.47
2:F:10:ALA:O	2:F:14:GLU:HB2	2.14	0.47
1:B:538:ILE:HD13	1:B:625:LEU:HD11	1.95	0.47
1:B:657:ILE:HG12	1:B:658:PRO:CD	2.44	0.47
1:B:752:LEU:HD23	1:B:752:LEU:C	2.35	0.47
1:C:514:ASP:HA	1:C:517:VAL:HG12	1.96	0.47
2:D:10:ALA:O	2:D:14:GLU:HB2	2.15	0.47
1:A:656:THR:O	1:A:755:ARG:NH1	2.47	0.47
1:C:657:ILE:HG13	1:C:759:GLN:HB3	1.93	0.47
1:A:445:ARG:CZ	1:A:471:TRP:CZ2	2.98	0.47
1:A:697:ILE:CG1	1:A:731:GLU:HB2	2.45	0.47
1:B:706:ASN:HB2	1:B:724:ARG:NH2	2.28	0.47
2:D:26:THR:HG22	2:D:64:ASP:HB3	1.95	0.47
1:A:673:SER:O	1:A:674:SER:HB2	2.15	0.47
1:A:743:PRO:HD2	1:B:544:SER:HB2	1.97	0.47
1:B:501:LEU:HD12	1:B:623:ASP:O	2.15	0.47
1:B:585:GLU:HB3	1:B:586:PHE:CD1	2.50	0.47
1:C:607:ASN:HD21	1:C:609:GLU:HB2	1.79	0.47
1:C:700:TYR:CD1	1:C:727:GLN:HB3	2.49	0.47
1:C:768:LYS:O	1:C:768:LYS:HG2	2.14	0.47
2:D:5:THR:O	2:D:8:GLN:HB2	2.15	0.47
1:A:504:ILE:HD13	1:A:537:GLY:HA3	1.96	0.47
1:A:629:ASN:HB3	1:A:632:TYR:CE2	2.49	0.47
1:B:407:HIS:H	1:B:407:HIS:CD2	2.31	0.47
1:C:415:GLU:C	1:C:417:GLY:H	2.18	0.47
2:F:8:GLN:HE21	2:F:8:GLN:CA	2.23	0.47
1:A:510:GLN:O	1:A:514:ASP:OD2	2.33	0.46
1:C:714:GLN:CA	1:C:714:GLN:NE2	2.73	0.46
2:E:97:ASN:ND2	2:E:99:TYR:HB2	2.30	0.46
1:A:657:ILE:HB	1:A:658:PRO:HD2	1.98	0.46
1:B:360:VAL:HG22	1:B:360:VAL:O	2.15	0.46
1:B:763:LEU:O	1:B:766:HIS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ASN:ND2	1:A:645:TRP:H	2.07	0.46
1:B:728:ALA:HA	1:B:731:GLU:CD	2.36	0.46
1:C:360:VAL:HG13	1:C:360:VAL:O	2.14	0.46
1:C:740:GLN:O	1:C:741:ILE:C	2.53	0.46
1:C:747:ASN:HA	1:C:750:GLN:HG2	1.98	0.46
2:D:129:ASP:OD1	2:D:132:GLY:N	2.43	0.46
1:A:434:LEU:CD1	1:A:445:ARG:NH1	2.78	0.46
1:B:345:THR:HB	1:B:491:ASP:HB3	1.97	0.46
1:B:773:PHE:O	1:B:775:LEU:N	2.49	0.46
1:C:406:ASP:C	1:C:406:ASP:OD1	2.54	0.46
1:C:635:ILE:O	1:C:636:ALA:C	2.53	0.46
1:C:714:GLN:NE2	1:C:717:LYS:HD2	2.31	0.46
1:C:761:GLN:HE21	1:C:761:GLN:CA	2.20	0.46
1:A:737:LYS:HA	1:A:737:LYS:HD3	1.84	0.46
1:A:791:GLU:CD	1:A:791:GLU:N	2.68	0.46
1:B:445:ARG:HG2	1:B:471:TRP:CZ3	2.50	0.46
2:D:24:ASP:O	2:D:26:THR:HG23	2.16	0.46
2:F:24:ASP:O	2:F:26:THR:HG23	2.15	0.46
1:B:723:PHE:CE1	1:B:782:PHE:HE2	2.34	0.46
1:C:481:VAL:O	1:C:484:VAL:HG23	2.15	0.46
1:C:494:LEU:HD23	1:C:497:LEU:HG	1.97	0.46
1:C:295:VAL:CG2	1:C:603:ILE:HG22	2.43	0.46
1:A:294:ASP:O	1:A:610:MET:CE	2.64	0.46
1:A:607:ASN:ND2	1:A:609:GLU:HB2	2.31	0.46
1:A:667:LEU:HA	1:A:670:ILE:CG2	2.46	0.46
1:A:722:ILE:CD1	1:A:764:LEU:HD23	2.41	0.46
1:B:363:TYR:O	1:B:365:PRO:HD3	2.16	0.46
1:B:454:GLN:HA	1:B:472:ARG:O	2.16	0.46
1:B:526:GLN:O	1:B:529:VAL:HG22	2.16	0.46
2:D:102:ALA:HB1	2:D:121:VAL:HG12	1.98	0.46
2:E:80:ASP:O	2:E:82:GLU:N	2.49	0.46
1:A:602:PHE:O	1:A:603:ILE:HD13	2.16	0.46
1:A:658:PRO:CB	1:A:662:GLU:HG2	2.46	0.46
1:B:712:PHE:HD2	1:B:716:LYS:HE2	1.81	0.46
1:B:732:ILE:O	1:B:732:ILE:HG22	2.16	0.46
1:C:722:ILE:CD1	1:C:764:LEU:HD23	2.40	0.46
2:E:24:ASP:O	2:E:26:THR:HG23	2.15	0.46
2:F:102:ALA:HB2	2:F:125:ILE:HG13	1.97	0.46
1:B:478:ALA:HB1	1:B:486:LYS:C	2.37	0.46
1:B:513:TRP:O	1:B:517:VAL:HG12	2.16	0.46
1:B:761:GLN:O	1:B:765:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:GLU:C	1:C:417:GLY:N	2.69	0.46
1:C:504:ILE:HD13	1:C:537:GLY:CA	2.46	0.46
1:A:525:LYS:HD3	2:D:124:MET:CE	2.45	0.46
1:A:505:LYS:C	1:A:507:GLN:H	2.19	0.46
1:A:555:GLN:O	1:A:559:ARG:HG2	2.15	0.46
2:F:114:GLU:O	2:F:114:GLU:HG3	2.14	0.46
1:A:549:LEU:HD13	1:A:554:LYS:HE2	1.97	0.45
1:A:736:LEU:HD21	1:A:749:PHE:CB	2.44	0.45
1:C:349:ASN:ND2	1:C:349:ASN:N	2.58	0.45
1:C:463:THR:HG22	1:C:464:VAL:N	2.30	0.45
1:B:650:THR:O	1:B:651:LYS:O	2.34	0.45
1:C:695:LYS:HD2	2:F:18:LEU:HB3	1.98	0.45
2:D:105:LEU:HD12	2:D:125:ILE:CD1	2.46	0.45
2:D:52:ILE:O	2:D:52:ILE:HG13	2.16	0.45
1:A:360:VAL:HG13	1:A:360:VAL:O	2.17	0.45
1:B:332:ASN:ND2	1:B:334:LEU:N	2.60	0.45
1:B:737:LYS:O	1:B:738:SER:O	2.34	0.45
1:C:440:GLN:HE21	1:C:441:VAL:HG23	1.76	0.45
1:C:401:ILE:HG21	1:C:485:LEU:HB3	1.99	0.45
2:F:76:MET:HA	2:F:79:THR:CG2	2.46	0.45
1:A:502:THR:O	1:A:505:LYS:HB3	2.16	0.45
1:A:712:PHE:CD2	1:A:716:LYS:HG2	2.52	0.45
1:B:400:LYS:HA	1:B:476:VAL:O	2.15	0.45
1:B:760:VAL:HG11	1:B:773:PHE:CE2	2.52	0.45
1:C:502:THR:O	1:C:505:LYS:HB3	2.16	0.45
1:C:499:PRO:HD3	1:C:552:TRP:CH2	2.52	0.45
1:C:540:ARG:NH1	1:C:582:ASP:OD1	2.46	0.45
1:C:631:SER:O	1:C:634:LYS:HB2	2.16	0.45
1:B:657:ILE:HG21	2:E:139:GLU:HG3	1.98	0.45
2:F:105:LEU:HD12	2:F:125:ILE:HD13	1.98	0.45
2:F:83:GLU:O	2:F:87:GLU:HG3	2.16	0.45
1:A:760:VAL:C	1:A:762:LEU:N	2.70	0.45
1:B:535:LYS:HA	1:B:535:LYS:CE	2.24	0.45
1:B:649:ILE:O	1:B:649:ILE:CG2	2.64	0.45
1:B:726:ILE:O	1:B:729:TYR:HB3	2.17	0.45
1:C:633:ASN:HD21	1:C:645:TRP:N	2.01	0.45
1:A:394:HIS:O	1:A:395:GLU:C	2.55	0.45
1:B:296:LEU:HD21	1:B:606:LYS:HE2	1.99	0.45
1:B:334:LEU:N	1:B:334:LEU:HD22	2.31	0.45
1:B:569:TYR:CZ	1:B:571:GLY:HA3	2.52	0.45
1:B:749:PHE:N	1:B:749:PHE:CD2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:GLN:O	1:C:762:LEU:HB3	2.17	0.45
1:A:438:ASN:ND2	1:A:438:ASN:C	2.69	0.45
1:A:516:VAL:O	1:A:517:VAL:C	2.55	0.45
1:B:654:ILE:HA	1:B:755:ARG:HG2	1.97	0.45
1:C:712:PHE:HB3	1:C:716:LYS:CG	2.47	0.45
2:E:118:ASP:O	2:E:122:ASP:OD2	2.35	0.45
1:A:313:ASP:HA	1:A:316:LYS:HE2	1.97	0.45
1:A:787:THR:O	1:A:787:THR:HG22	2.16	0.45
1:B:697:ILE:HD13	1:B:732:ILE:CD1	2.46	0.45
1:C:636:ALA:O	1:C:640:LYS:HA	2.17	0.45
1:A:668:SER:HA	2:D:14:GLU:HG3	1.99	0.45
2:E:8:GLN:HE21	2:E:8:GLN:CA	2.21	0.45
2:F:118:ASP:O	2:F:122:ASP:OD2	2.35	0.45
2:F:93:ASP:OD1	2:F:97:ASN:OD1	2.35	0.45
1:A:712:PHE:CE2	1:A:716:LYS:NZ	2.85	0.45
1:B:732:ILE:O	1:B:735:VAL:HG12	2.17	0.45
1:B:735:VAL:HG22	1:B:738:SER:HB2	1.98	0.45
1:B:780:LEU:HB3	1:B:782:PHE:HE1	1.79	0.45
1:C:742:ALA:HB3	1:C:745:TYR:CG	2.52	0.45
1:C:753:LYS:HB3	1:C:753:LYS:HZ3	1.82	0.45
2:E:105:LEU:HD12	2:E:125:ILE:HD13	1.98	0.45
1:B:418:ILE:O	1:B:419:ILE:HG23	2.17	0.45
1:B:735:VAL:HG13	1:B:735:VAL:O	2.16	0.45
1:C:670:ILE:HG23	1:C:745:TYR:CE1	2.52	0.45
1:A:695:LYS:HD2	2:D:19:PHE:HB2	1.97	0.45
2:E:76:MET:HA	2:E:79:THR:CG2	2.47	0.45
1:A:415:GLU:C	1:A:417:GLY:H	2.19	0.44
1:A:714:GLN:NE2	1:A:717:LYS:HD2	2.32	0.44
1:A:742:ALA:HB3	1:A:745:TYR:CG	2.52	0.44
1:B:504:ILE:HD12	1:B:537:GLY:HA2	1.98	0.44
1:B:762:LEU:O	1:B:766:HIS:HB2	2.17	0.44
1:A:462:ILE:CG1	1:A:466:GLY:HA2	2.46	0.44
1:A:648:PRO:HA	1:A:651:LYS:CD	2.46	0.44
1:B:730:ASN:HD21	1:B:734:ASN:CB	2.29	0.44
1:B:729:TYR:HE2	1:B:773:PHE:CD1	2.34	0.44
1:C:736:LEU:HD21	1:C:749:PHE:CB	2.45	0.44
2:F:27:ILE:HB	2:F:31:GLU:CG	2.47	0.44
1:A:298:GLY:O	1:A:301:ALA:N	2.50	0.44
1:A:318:ILE:H	1:A:318:ILE:HD12	1.82	0.44
1:A:712:PHE:CD2	1:A:716:LYS:NZ	2.85	0.44
1:A:724:ARG:HA	1:A:727:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ILE:HB	1:B:477:MET:HB2	1.99	0.44
2:E:115:LYS:NZ	2:E:115:LYS:HB3	2.33	0.44
2:E:83:GLU:O	2:E:87:GLU:HG3	2.17	0.44
2:F:129:ASP:OD1	2:F:130:ILE:N	2.50	0.44
1:A:437:SER:C	1:A:439:ASN:H	2.21	0.44
1:A:463:THR:HG22	1:A:464:VAL:N	2.32	0.44
1:A:767:GLN:HE21	1:A:767:GLN:HB3	1.70	0.44
1:B:730:ASN:O	1:B:730:ASN:ND2	2.50	0.44
1:C:760:VAL:C	1:C:762:LEU:N	2.71	0.44
1:C:768:LYS:HD2	1:C:797:ILE:O	2.17	0.44
2:D:27:ILE:HB	2:D:31:GLU:CG	2.47	0.44
2:E:80:ASP:C	2:E:82:GLU:N	2.71	0.44
2:F:143:GLN:HA	2:F:143:GLN:OE1	2.17	0.44
1:A:494:LEU:HD23	1:A:497:LEU:HG	1.98	0.44
1:A:635:ILE:O	1:A:636:ALA:C	2.52	0.44
1:A:712:PHE:HB3	1:A:716:LYS:CG	2.47	0.44
1:A:724:ARG:O	1:A:727:GLN:HB2	2.17	0.44
1:B:789:ASN:ND2	1:B:793:PHE:HB2	2.32	0.44
1:C:316:LYS:HG2	1:C:600:GLY:CA	2.47	0.44
1:C:718:ARG:O	1:C:722:ILE:HG13	2.17	0.44
2:E:92:PHE:CE2	2:E:108:VAL:HG11	2.52	0.44
1:A:415:GLU:O	1:A:417:GLY:N	2.51	0.44
1:A:700:TYR:CD1	1:A:727:GLN:HB3	2.53	0.44
1:B:297:LYS:O	1:B:298:GLY:O	2.36	0.44
1:C:325:TYR:HB2	1:C:498:ALA:HB3	1.98	0.44
1:C:629:ASN:HD21	1:C:631:SER:HB2	1.81	0.44
1:C:724:ARG:HA	1:C:727:GLN:HE21	1.82	0.44
1:C:733:GLU:O	1:C:737:LYS:HE2	2.18	0.44
1:A:631:SER:O	1:A:634:LYS:HB2	2.18	0.44
1:B:729:TYR:HD1	1:B:729:TYR:O	2.01	0.44
1:C:313:ASP:O	1:C:316:LYS:HB2	2.17	0.44
2:D:118:ASP:O	2:D:122:ASP:OD2	2.35	0.44
2:F:5:THR:N	2:F:8:GLN:HG3	2.33	0.44
1:B:565:LYS:C	1:B:567:THR:N	2.71	0.44
1:C:724:ARG:O	1:C:727:GLN:HB2	2.17	0.44
1:C:777:TYR:O	1:C:777:TYR:CG	2.70	0.44
2:D:143:GLN:OE1	2:D:143:GLN:HA	2.18	0.44
2:F:5:THR:N	2:F:8:GLN:CG	2.80	0.44
1:A:617:LYS:HD2	1:A:617:LYS:O	2.18	0.44
1:A:697:ILE:HG13	1:A:731:GLU:HB3	2.00	0.44
1:B:514:ASP:O	1:B:516:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ASN:C	1:C:323:ASN:HD22	2.21	0.44
1:C:668:SER:HB2	2:F:14:GLU:HG3	1.99	0.44
1:B:713:SER:O	1:B:716:LYS:N	2.50	0.43
1:B:762:LEU:O	1:B:766:HIS:N	2.51	0.43
1:C:607:ASN:ND2	1:C:609:GLU:HB2	2.33	0.43
1:B:327:LEU:N	1:B:327:LEU:CD1	2.81	0.43
1:B:432:TYR:CD2	1:B:447:SER:HA	2.54	0.43
1:B:764:LEU:O	1:B:768:LYS:HB2	2.17	0.43
2:E:81:SER:O	2:E:82:GLU:C	2.56	0.43
1:A:777:TYR:O	1:A:777:TYR:CG	2.72	0.43
1:B:295:VAL:HG13	1:B:610:MET:CE	2.48	0.43
1:B:427:ASP:C	1:B:429:GLY:H	2.21	0.43
1:B:748:TYR:HD2	1:B:749:PHE:HD2	1.64	0.43
1:C:438:ASN:ND2	1:C:438:ASN:C	2.72	0.43
1:C:672:ARG:C	1:C:674:SER:H	2.21	0.43
2:E:103:ALA:O	2:E:106:ARG:HB3	2.18	0.43
2:E:27:ILE:HB	2:E:31:GLU:CG	2.47	0.43
1:A:445:ARG:HG3	1:A:471:TRP:CE2	2.52	0.43
2:F:81:SER:O	2:F:82:GLU:C	2.56	0.43
1:A:307:LEU:N	1:A:307:LEU:HD12	2.33	0.43
1:A:401:ILE:HG21	1:A:485:LEU:HB3	2.00	0.43
1:A:659:THR:HG22	1:A:662:GLU:H	1.81	0.43
1:B:651:LYS:HB3	1:B:652:ALA:H	1.53	0.43
1:B:697:ILE:HD13	1:B:732:ILE:HD13	2.01	0.43
1:B:751:TYR:O	1:B:754:GLU:N	2.52	0.43
2:F:88:ALA:O	2:F:89:PHE:C	2.56	0.43
1:A:353:LYS:HB3	1:A:372:LYS:HE2	2.01	0.43
1:A:660:SER:O	1:A:663:PHE:HB3	2.18	0.43
1:B:322:LEU:HD11	1:B:559:ARG:HD3	2.00	0.43
1:B:791:GLU:HG3	1:B:792:VAL:H	1.82	0.43
1:C:331:VAL:O	1:C:332:ASN:C	2.55	0.43
1:C:505:LYS:C	1:C:507:GLN:N	2.72	0.43
2:E:129:ASP:OD1	2:E:130:ILE:N	2.52	0.43
1:A:340:LYS:C	1:A:342:GLY:N	2.71	0.43
1:A:617:LYS:HD2	1:A:618:ASN:OD1	2.19	0.43
1:B:316:LYS:HE3	1:B:602:PHE:CZ	2.53	0.43
1:B:461:LYS:C	1:B:462:ILE:HG13	2.38	0.43
1:C:694:VAL:HG23	1:C:695:LYS:N	2.23	0.43
1:A:558:ASP:O	1:A:562:GLU:HG3	2.19	0.43
1:A:727:GLN:O	1:A:730:ASN:HB3	2.19	0.43
1:B:549:LEU:HD13	1:B:578:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:GLN:HG3	1:B:765:THR:HG21	2.01	0.43
2:E:7:GLU:O	2:E:11:GLU:HG3	2.19	0.43
2:F:102:ALA:HB1	2:F:121:VAL:HG12	2.01	0.43
1:A:349:ASN:ND2	1:A:349:ASN:H	1.95	0.43
1:A:391:ILE:CD1	1:A:399:GLY:HA2	2.49	0.43
1:B:311:HIS:CD2	1:B:564:VAL:HB	2.54	0.43
1:B:375:GLY:HA2	1:B:464:VAL:CG1	2.49	0.43
1:B:622:LYS:HB3	1:B:624:TYR:HD1	1.84	0.43
1:C:298:GLY:O	1:C:299:GLU:C	2.57	0.43
1:C:619:ILE:C	1:C:621:GLY:H	2.22	0.43
1:C:628:PHE:CD1	1:C:628:PHE:C	2.92	0.43
1:C:727:GLN:O	1:C:730:ASN:HB3	2.19	0.43
1:A:730:ASN:OD1	1:A:782:PHE:CD2	2.72	0.43
1:B:294:ASP:HB3	1:B:610:MET:HE3	2.00	0.43
1:B:318:ILE:CG2	1:B:322:LEU:HD12	2.48	0.43
1:B:597:ASN:OD1	1:B:600:GLY:N	2.52	0.43
1:C:504:ILE:HD11	1:C:625:LEU:HD22	1.98	0.43
1:A:527:LYS:HA	2:D:145:MET:SD	2.59	0.43
2:E:20:ASP:C	2:E:22:ASP:H	2.21	0.43
1:A:657:ILE:HG23	1:A:759:GLN:HG2	2.01	0.42
1:B:478:ALA:CB	1:B:486:LYS:O	2.65	0.42
1:B:657:ILE:CG1	1:B:658:PRO:CD	2.97	0.42
1:C:509:PRO:HD2	1:C:536:TYR:CE2	2.54	0.42
2:F:128:ALA:HB2	2:F:144:MET:HG3	2.01	0.42
1:A:747:ASN:HA	1:A:750:GLN:HG2	2.00	0.42
1:A:794:GLN:CA	1:A:794:GLN:HE21	2.32	0.42
1:B:752:LEU:O	1:B:752:LEU:HD23	2.19	0.42
1:C:639:ASN:HD22	1:C:640:LYS:N	2.18	0.42
2:D:13:LYS:HG3	2:D:65:PHE:HE2	1.82	0.42
2:D:55:VAL:HG13	2:D:56:ASP:H	1.84	0.42
2:D:80:ASP:C	2:D:82:GLU:N	2.72	0.42
2:D:80:ASP:O	2:D:82:GLU:N	2.52	0.42
2:F:107:HIS:O	2:F:111:ASN:ND2	2.48	0.42
2:F:115:LYS:HB3	2:F:115:LYS:NZ	2.34	0.42
1:A:485:LEU:HA	1:A:485:LEU:HD12	1.92	0.42
1:A:636:ALA:O	1:A:640:LYS:HA	2.19	0.42
1:B:642:TYR:HE2	1:B:644:GLU:OE2	2.02	0.42
1:C:323:ASN:C	1:C:323:ASN:ND2	2.72	0.42
1:C:340:LYS:C	1:C:342:GLY:N	2.71	0.42
1:C:623:ASP:OD2	2:F:107:HIS:HD2	2.02	0.42
1:C:795:LYS:O	1:C:798:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:GLU:O	2:F:11:GLU:HG3	2.19	0.42
1:A:415:GLU:C	1:A:417:GLY:N	2.73	0.42
1:B:739:LYS:O	1:B:741:ILE:HG13	2.20	0.42
1:A:462:ILE:HD12	1:A:467:GLU:O	2.19	0.42
1:A:667:LEU:O	1:A:670:ILE:HG22	2.18	0.42
1:C:307:LEU:N	1:C:307:LEU:HD12	2.33	0.42
1:C:440:GLN:CD	1:C:440:GLN:H	2.23	0.42
1:C:712:PHE:CD2	1:C:716:LYS:HG2	2.55	0.42
1:C:753:LYS:NZ	1:C:753:LYS:CB	2.82	0.42
2:F:80:ASP:C	2:F:82:GLU:N	2.72	0.42
1:B:317:LYS:O	1:B:320:ARG:HG2	2.20	0.42
1:B:648:PRO:C	1:B:650:THR:N	2.72	0.42
1:C:456:LYS:HD2	1:C:470:ASN:OD1	2.20	0.42
1:C:652:ALA:O	1:C:654:ILE:N	2.52	0.42
1:A:323:ASN:ND2	1:A:323:ASN:C	2.73	0.42
1:A:697:ILE:CG1	1:A:731:GLU:CB	2.98	0.42
1:B:415:GLU:C	1:B:417:GLY:H	2.22	0.42
1:B:712:PHE:HB3	1:B:716:LYS:HG2	2.01	0.42
1:C:298:GLY:O	1:C:301:ALA:N	2.53	0.42
2:E:37:ARG:HG2	2:E:41:GLN:O	2.19	0.42
2:F:105:LEU:O	2:F:109:MET:HG2	2.20	0.42
2:F:117:THR:O	2:F:121:VAL:HG23	2.19	0.42
1:A:456:LYS:HB2	1:A:470:ASN:O	2.19	0.42
1:A:509:PRO:O	1:A:511:LYS:N	2.46	0.42
1:A:559:ARG:O	1:A:562:GLU:HB2	2.19	0.42
1:A:667:LEU:C	1:A:670:ILE:HG22	2.40	0.42
1:B:508:ILE:CG2	1:B:509:PRO:HD2	2.48	0.42
1:B:614:PHE:CD2	1:B:614:PHE:C	2.92	0.42
1:C:695:LYS:CD	2:F:18:LEU:HB3	2.49	0.42
2:D:115:LYS:NZ	2:D:115:LYS:HB3	2.32	0.42
2:F:32:LEU:O	2:F:36:MET:HG3	2.20	0.42
2:F:37:ARG:HG2	2:F:41:GLN:O	2.20	0.42
1:A:797:ILE:C	1:A:797:ILE:HD12	2.40	0.42
1:B:761:GLN:HA	1:B:761:GLN:NE2	2.35	0.42
1:C:639:ASN:C	1:C:639:ASN:ND2	2.73	0.42
1:C:690:LYS:HE3	1:C:694:VAL:HG22	2.02	0.42
2:E:105:LEU:O	2:E:109:MET:HG2	2.20	0.42
2:F:80:ASP:O	2:F:82:GLU:N	2.52	0.42
1:A:499:PRO:HD3	1:A:552:TRP:CH2	2.54	0.42
1:B:313:ASP:O	1:B:314:ALA:C	2.55	0.42
1:C:370:LEU:HD11	1:C:455:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:GLN:O	1:C:377:GLN:HG2	2.19	0.42
1:C:633:ASN:HD22	1:C:644:GLU:HA	1.85	0.42
1:C:751:TYR:O	1:C:754:GLU:HB3	2.20	0.42
1:C:761:GLN:NE2	1:C:761:GLN:HA	2.29	0.42
2:E:129:ASP:OD1	2:E:132:GLY:N	2.47	0.42
2:E:29:THR:O	2:E:29:THR:HG22	2.20	0.42
2:F:7:GLU:HA	2:F:10:ALA:CB	2.47	0.42
1:A:298:GLY:O	1:A:299:GLU:C	2.59	0.41
1:B:515:LYS:HB2	1:B:515:LYS:HE3	1.92	0.41
1:B:543:ASP:OD1	1:B:544:SER:N	2.53	0.41
1:B:657:ILE:HB	1:B:705:TYR:HE1	1.85	0.41
1:C:670:ILE:O	1:C:745:TYR:HE1	2.03	0.41
2:E:107:HIS:O	2:E:111:ASN:ND2	2.46	0.41
1:B:327:LEU:N	1:B:327:LEU:HD12	2.35	0.41
1:C:655:ASN:N	1:C:655:ASN:ND2	2.63	0.41
1:C:712:PHE:CE2	1:C:716:LYS:NZ	2.88	0.41
1:A:360:VAL:O	1:A:360:VAL:HG22	2.20	0.41
1:C:619:ILE:C	1:C:621:GLY:N	2.74	0.41
2:E:92:PHE:CZ	2:E:108:VAL:HG11	2.56	0.41
2:F:106:ARG:O	2:F:110:THR:HG23	2.20	0.41
1:A:794:GLN:NE2	1:A:794:GLN:HA	2.36	0.41
1:B:313:ASP:C	1:B:315:PHE:N	2.74	0.41
1:B:366:PHE:CD1	1:B:477:MET:HE2	2.51	0.41
1:B:505:LYS:C	1:B:507:GLN:N	2.73	0.41
1:B:518:ASN:C	1:B:519:THR:HG22	2.40	0.41
1:B:764:LEU:CD2	1:B:768:LYS:HD3	2.48	0.41
1:C:295:VAL:CG2	1:C:603:ILE:CG2	2.88	0.41
1:C:794:GLN:CA	1:C:794:GLN:HE21	2.33	0.41
2:D:103:ALA:O	2:D:106:ARG:HB3	2.20	0.41
2:D:29:THR:HG22	2:D:29:THR:O	2.20	0.41
1:A:445:ARG:CZ	1:A:471:TRP:HZ2	2.33	0.41
1:A:586:PHE:CE2	1:A:638:GLY:HA3	2.55	0.41
1:A:659:THR:HG23	1:A:661:ALA:N	2.36	0.41
1:A:695:LYS:CD	2:D:18:LEU:HB3	2.50	0.41
1:B:470:ASN:CG	1:B:471:TRP:H	2.24	0.41
1:B:607:ASN:ND2	1:B:609:GLU:HB2	2.36	0.41
1:C:712:PHE:CD2	1:C:716:LYS:NZ	2.88	0.41
2:D:106:ARG:O	2:D:110:THR:HG23	2.20	0.41
2:D:117:THR:OG1	2:D:120:GLU:HG3	2.20	0.41
2:F:20:ASP:C	2:F:22:ASP:H	2.22	0.41
1:A:295:VAL:HG21	1:A:603:ILE:HG23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASN:HD22	1:A:323:ASN:C	2.23	0.41
1:A:649:ILE:HG22	1:A:649:ILE:O	2.20	0.41
1:A:662:GLU:O	1:A:666:ASN:OD1	2.38	0.41
1:A:781:ASN:HB2	1:A:789:ASN:OD1	2.20	0.41
1:B:299:GLU:HB3	1:B:303:LYS:NZ	2.36	0.41
1:B:305:SER:O	1:B:331:VAL:HB	2.20	0.41
1:B:519:THR:N	1:B:520:PRO:HD2	2.36	0.41
1:B:714:GLN:OE1	1:B:718:ARG:NH2	2.54	0.41
1:C:509:PRO:C	1:C:511:LYS:H	2.21	0.41
1:B:649:ILE:CD1	2:E:86:ARG:HG3	2.50	0.41
1:B:732:ILE:O	1:B:735:VAL:CG1	2.69	0.41
1:B:778:LYS:C	1:B:780:LEU:H	2.23	0.41
2:E:7:GLU:HA	2:E:10:ALA:CB	2.47	0.41
1:B:332:ASN:C	1:B:332:ASN:ND2	2.72	0.41
1:B:401:ILE:HD11	1:B:487:PRO:HD3	2.02	0.41
1:B:529:VAL:HG23	1:B:530:THR:N	2.36	0.41
1:C:510:GLN:CG	1:C:510:GLN:O	2.64	0.41
1:C:722:ILE:HG12	1:C:763:LEU:HB2	2.03	0.41
2:E:128:ALA:HB2	2:E:144:MET:HG3	2.02	0.41
2:F:103:ALA:O	2:F:106:ARG:HB3	2.20	0.41
1:A:318:ILE:H	1:A:318:ILE:CD1	2.34	0.41
1:B:784:GLU:OE1	1:B:788:ASP:HB3	2.21	0.41
2:D:7:GLU:HA	2:D:10:ALA:CB	2.46	0.41
2:E:32:LEU:O	2:E:36:MET:HG3	2.21	0.41
1:A:331:VAL:O	1:A:332:ASN:C	2.58	0.41
1:B:320:ARG:C	1:B:322:LEU:N	2.73	0.41
1:B:748:TYR:C	1:B:750:GLN:N	2.75	0.41
1:B:729:TYR:CE2	1:B:773:PHE:CE1	3.05	0.41
1:C:505:LYS:O	1:C:507:GLN:N	2.54	0.41
1:C:709:ASN:C	1:C:711:ILE:H	2.24	0.41
1:C:732:ILE:HG21	1:C:753:LYS:HG3	2.02	0.41
2:D:7:GLU:O	2:D:11:GLU:HG3	2.21	0.41
2:D:81:SER:O	2:D:82:GLU:C	2.60	0.41
2:F:5:THR:O	2:F:9:ILE:HG13	2.21	0.41
1:A:760:VAL:O	1:A:762:LEU:N	2.54	0.41
1:B:297:LYS:HZ1	1:B:601:GLU:CB	2.30	0.41
1:B:509:PRO:O	1:B:511:LYS:N	2.54	0.41
1:B:597:ASN:OD1	1:B:599:GLU:HB2	2.21	0.41
1:B:793:PHE:C	1:B:795:LYS:N	2.74	0.41
1:A:621:GLY:O	1:A:622:LYS:HD2	2.20	0.40
1:B:546:LYS:CB	1:B:549:LEU:HD22	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:HD2	1:B:590:ASP:OD2	2.22	0.40
1:B:730:ASN:HD21	1:B:734:ASN:HB3	1.85	0.40
1:C:532:LEU:HD23	1:C:532:LEU:HA	1.85	0.40
1:C:797:ILE:HD12	1:C:797:ILE:C	2.41	0.40
2:D:32:LEU:O	2:D:36:MET:HG3	2.20	0.40
2:E:117:THR:O	2:E:121:VAL:HG23	2.20	0.40
1:B:538:ILE:O	1:B:540:ARG:HD3	2.22	0.40
1:C:492:TYR:CD2	1:C:574:VAL:HG13	2.57	0.40
1:C:654:ILE:HG22	1:C:655:ASN:ND2	2.35	0.40
1:A:407:HIS:H	1:A:407:HIS:CD2	2.34	0.40
1:A:500:SER:HA	1:A:624:TYR:HA	2.03	0.40
1:A:525:LYS:O	1:A:529:VAL:HG23	2.22	0.40
1:A:749:PHE:C	1:A:751:TYR:N	2.74	0.40
1:A:722:ILE:HG21	1:A:764:LEU:HD21	2.03	0.40
1:B:459:GLU:C	1:B:461:LYS:N	2.75	0.40
1:B:589:LYS:HZ1	1:B:608:TRP:CB	2.35	0.40
1:B:728:ALA:C	1:B:730:ASN:N	2.75	0.40
1:B:753:LYS:C	1:B:755:ARG:N	2.74	0.40
1:A:629:ASN:HD21	1:A:631:SER:HB2	1.86	0.40
1:B:776:LEU:HD13	1:B:779:GLN:NE2	2.36	0.40
1:C:602:PHE:O	1:C:603:ILE:HD13	2.21	0.40
1:C:797:ILE:CG1	1:C:798:ASP:N	2.84	0.40
1:B:525:LYS:NZ	2:E:114:GLU:OE2	2.44	0.40
2:F:29:THR:O	2:F:29:THR:HG22	2.21	0.40
1:B:390:SER:HB3	1:B:398:ILE:HG21	2.02	0.40
1:C:391:ILE:CD1	1:C:399:GLY:HA2	2.52	0.40
1:C:397:GLU:O	1:C:398:ILE:HD13	2.22	0.40
1:C:536:TYR:O	1:C:552:TRP:HD1	2.05	0.40
1:C:784:GLU:N	1:C:784:GLU:OE1	2.55	0.40
2:D:76:MET:HA	2:D:79:THR:HG23	2.04	0.40
1:B:762:LEU:HD21	2:E:135:GLN:NE2	2.36	0.40
2:E:77:LYS:HD2	2:E:77:LYS:HA	1.96	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	479/510 (94%)	405 (85%)	63 (13%)	11 (2%)	7	32
1	B	461/510 (90%)	352 (76%)	81 (18%)	28 (6%)	2	8
1	C	499/510 (98%)	415 (83%)	66 (13%)	18 (4%)	4	19
2	D	141/144 (98%)	119 (84%)	17 (12%)	5 (4%)	4	20
2	E	141/144 (98%)	118 (84%)	18 (13%)	5 (4%)	4	20
2	F	141/144 (98%)	118 (84%)	18 (13%)	5 (4%)	4	20
All	All	1862/1962 (95%)	1527 (82%)	263 (14%)	72 (4%)	3	17

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	741	ILE
1	B	299	GLU
1	B	526	GLN
1	B	544	SER
1	B	571	GLY
1	B	651	LYS
1	B	702	SER
1	B	708	ALA
1	B	713	SER
1	C	520	PRO
1	C	741	ILE
1	A	294	ASP
1	A	298	GLY
1	A	510	GLN
1	A	775	LEU
1	B	298	GLY
1	B	377	GLN
1	B	460	GLY
1	B	510	GLN
1	B	515	LYS
1	B	566	TYR
1	B	732	ILE
1	C	298	GLY
1	C	299	GLU
1	C	510	GLN
1	C	578	GLY

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Mol	Chain	Res	Type
1	C	675	ASN
1	C	694	VAL
1	C	775	LEU
1	C	787	THR
2	E	93	ASP
1	A	299	GLU
1	A	416	ASN
1	A	783	THR
1	B	537	GLY
1	B	542	PRO
1	B	735	VAL
1	B	738	SER
1	B	776	LEU
2	D	76	MET
2	D	81	SER
2	D	93	ASP
2	E	76	MET
2	E	81	SER
2	F	76	MET
2	F	93	ASP
1	A	377	GLN
1	B	314	ALA
1	B	704	TYR
1	C	416	ASN
1	C	506	LYS
1	C	692	GLU
2	F	81	SER
1	B	321	GLU
1	B	578	GLY
1	B	630	ARG
1	B	694	VAL
1	B	712	PHE
1	C	653	LYS
1	C	662	GLU
1	C	677	GLY
1	C	719	LYS
2	D	74	ARG
2	E	74	ARG
2	F	74	ARG
1	A	578	GLY
1	B	519	THR
1	A	517	VAL

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Mol	Chain	Res	Type
2	D	52	ILE
2	E	52	ILE
2	F	52	ILE
1	C	293	ILE

### 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	433/455 (95%)	393 (91%)	40 (9%)	11	35
1	B	414/455 (91%)	377 (91%)	37 (9%)	11	37
1	C	448/455 (98%)	409 (91%)	39 (9%)	12	38
2	D	121/123 (98%)	117 (97%)	4 (3%)	43	77
2	E	121/123 (98%)	117 (97%)	4 (3%)	43	77
2	F	121/123 (98%)	116 (96%)	5 (4%)	35	71
All	All	1658/1734 (96%)	1529 (92%)	129 (8%)	15	44

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	349	ASN
1	A	373	LYS
1	A	385	LEU
1	A	388	LYS
1	A	401	ILE
1	A	406	ASP
1	A	434	LEU
1	A	438	ASN
1	A	440	GLN
1	A	445	ARG
1	A	455	TYR
1	A	457	THR
1	A	471	TRP

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Mol	Chain	Res	Type
1	A	484	VAL
1	A	485	LEU
1	A	549	LEU
1	A	558	ASP
1	A	574	VAL
1	A	618	ASN
1	A	629	ASN
1	A	631	SER
1	A	639	ASN
1	A	651	LYS
1	A	662	GLU
1	A	668	SER
1	A	670	ILE
1	A	673	SER
1	A	714	GLN
1	A	715	GLU
1	A	737	LYS
1	A	745	TYR
1	A	761	GLN
1	A	767	GLN
1	A	775	LEU
1	A	779	GLN
1	A	780	LEU
1	A	789	ASN
1	A	791	GLU
1	A	797	ILE
1	B	320	ARG
1	B	327	LEU
1	B	332	ASN
1	B	336	THR
1	B	341	SER
1	B	353	LYS
1	B	354	SER
1	B	378	LEU
1	B	397	GLU
1	B	415	GLU
1	B	434	LEU
1	B	437	SER
1	B	447	SER
1	B	480	ASN
1	B	510	GLN
1	B	521	ASN

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Mol	Chain	Res	Type
1	B	524	GLU
1	B	526	GLN
1	B	540	ARG
1	B	545	THR
1	B	551	ASN
1	B	552	TRP
1	B	557	LEU
1	B	570	THR
1	B	574	VAL
1	B	585	GLU
1	B	629	ASN
1	B	631	SER
1	B	639	ASN
1	B	646	THR
1	B	712	PHE
1	B	729	TYR
1	B	730	ASN
1	B	744	GLU
1	B	775	LEU
1	B	784	GLU
1	B	787	THR
1	C	317	LYS
1	C	323	ASN
1	C	349	ASN
1	C	373	LYS
1	C	385	LEU
1	C	388	LYS
1	C	401	ILE
1	C	406	ASP
1	C	419	ILE
1	C	434	LEU
1	C	438	ASN
1	C	440	GLN
1	C	455	TYR
1	C	457	THR
1	C	484	VAL
1	C	485	LEU
1	C	514	ASP
1	C	549	LEU
1	C	558	ASP
1	C	574	VAL
1	C	618	ASN

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Mol	Chain	Res	Type
1	C	629	ASN
1	C	639	ASN
1	C	650	THR
1	C	659	THR
1	C	666	ASN
1	C	714	GLN
1	C	715	GLU
1	C	737	LYS
1	C	745	TYR
1	C	761	GLN
1	C	767	GLN
1	C	775	LEU
1	C	779	GLN
1	C	780	LEU
1	C	784	GLU
1	C	789	ASN
1	C	791	GLU
1	C	797	ILE
2	D	16	PHE
2	D	64	ASP
2	D	76	MET
2	D	135	GLN
2	E	16	PHE
2	E	64	ASP
2	E	76	MET
2	E	135	GLN
2	F	16	PHE
2	F	64	ASP
2	F	76	MET
2	F	135	GLN
2	F	146	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	337	ASN
1	A	349	ASN
1	A	416	ASN
1	A	438	ASN
1	A	507	GLN
1	A	510	GLN

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Mol	Chain	Res	Type
1	A	518	ASN
1	A	531	ASN
1	A	553	GLN
1	A	555	GLN
1	A	581	GLN
1	A	607	ASN
1	A	629	ASN
1	A	633	ASN
1	A	639	ASN
1	A	655	ASN
1	A	666	ASN
1	A	706	ASN
1	A	714	GLN
1	A	727	GLN
1	A	781	ASN
1	A	789	ASN
1	A	794	GLN
1	B	311	HIS
1	B	332	ASN
1	B	351	HIS
1	B	368	GLN
1	B	377	GLN
1	B	407	HIS
1	B	451	ASN
1	B	507	GLN
1	B	518	ASN
1	B	521	ASN
1	B	526	GLN
1	B	551	ASN
1	B	553	GLN
1	B	607	ASN
1	B	629	ASN
1	B	639	ASN
1	B	655	ASN
1	B	727	GLN
1	B	730	ASN
1	B	758	ASN
1	B	759	GLN
1	B	761	GLN
1	B	794	GLN
1	C	323	ASN
1	C	337	ASN

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Mol	Chain	Res	Type
1	C	349	ASN
1	C	407	HIS
1	C	416	ASN
1	C	438	ASN
1	C	507	GLN
1	C	510	GLN
1	C	518	ASN
1	C	526	GLN
1	C	553	GLN
1	C	555	GLN
1	C	581	GLN
1	C	607	ASN
1	C	629	ASN
1	C	633	ASN
1	C	639	ASN
1	C	655	ASN
1	C	666	ASN
1	C	706	ASN
1	C	714	GLN
1	C	727	GLN
1	C	761	GLN
1	C	781	ASN
1	C	789	ASN
1	C	794	GLN
2	D	8	GLN
2	E	8	GLN
2	E	135	GLN
2	F	8	GLN
2	F	107	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
3	SO4	A	1001	-	4,4,4	1.67	1 (25%)	6,6,6	0.58	0
3	SO4	C	1003	-	4,4,4	1.89	2 (50%)	6,6,6	1.03	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
3	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1003	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	SO4	O3-S	2.03	1.64	1.47
3	C	1003	SO4	O2-S	2.07	1.56	1.45
3	A	1001	SO4	O2-S	2.18	1.57	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	485/510 (95%)	0.18	13 (2%)	55 36	35, 71, 148, 169	16 (3%)
1	B	459/510 (90%)	0.40	40 (8%)	11 6	33, 69, 160, 167	12 (2%)
1	C	491/510 (96%)	0.32	32 (6%)	20 11	34, 74, 148, 169	19 (3%)
2	D	143/144 (99%)	1.31	38 (26%)	1 0	53, 145, 174, 176	0
2	E	143/144 (99%)	1.58	48 (33%)	0 0	55, 146, 174, 176	0
2	F	143/144 (99%)	1.49	38 (26%)	1 0	56, 146, 174, 176	0
All	All	1864/1962 (95%)	0.57	209 (11%)	6 3	33, 77, 168, 176	47 (2%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	19	PHE	11.6
1	B	776	LEU	8.4
2	E	21	LYS	7.9
2	F	29	THR	7.6
2	E	76	MET	7.2
1	B	740	GLN	7.1
1	A	779	GLN	7.1
2	D	19	PHE	7.0
2	F	63	ILE	6.6
1	B	780	LEU	6.6
2	D	77	LYS	6.4
2	E	19	PHE	6.1
1	B	739	LYS	5.9
2	F	55	VAL	5.9
2	E	61	GLY	5.9
2	D	65	PHE	5.6
1	B	773	PHE	5.6
2	F	51	MET	5.6
1	B	779	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
2	D	76	MET	5.5
2	E	71	MET	5.4
1	C	744	GLU	5.4
2	E	55	VAL	5.3
1	B	741	ILE	5.3
2	E	59	GLY	5.2
1	A	782	PHE	5.1
2	E	121	VAL	5.0
1	B	736	LEU	5.0
2	F	73	ALA	5.0
1	C	779	GLN	5.0
2	F	77	LYS	4.9
2	F	76	MET	4.9
1	B	778	LYS	4.9
2	F	60	ASN	4.9
2	E	5	THR	4.8
1	B	749	PHE	4.8
2	F	30	LYS	4.7
2	E	77	LYS	4.7
2	D	57	ALA	4.7
2	D	30	LYS	4.6
1	B	697	ILE	4.5
2	D	53	ASN	4.4
2	E	72	MET	4.4
2	F	12	PHE	4.4
2	F	22	ASP	4.4
2	E	6	GLU	4.4
2	F	57	ALA	4.4
2	E	60	ASN	4.4
2	F	28	THR	4.3
1	B	782	PHE	4.3
2	F	32	LEU	4.3
2	D	16	PHE	4.3
2	E	53	ASN	4.2
2	D	55	VAL	4.2
2	E	69	LEU	4.2
2	D	58	ASP	4.2
2	F	46	ALA	4.1
1	C	741	ILE	4.1
1	C	742	ALA	4.0
1	C	766	HIS	4.0
1	B	658	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	56	ASP	4.0
1	C	776	LEU	4.0
2	F	62	THR	3.9
2	D	48	LEU	3.9
2	E	47	GLU	3.9
2	D	69	LEU	3.9
2	D	79	THR	3.8
1	B	354	SER	3.8
2	E	66	PRO	3.8
1	B	787	THR	3.8
2	D	21	LYS	3.8
2	F	20	ASP	3.8
2	F	33	GLY	3.8
1	C	689	ALA	3.8
1	B	705	TYR	3.7
2	E	54	GLU	3.7
2	E	80	ASP	3.7
2	E	62	THR	3.7
2	E	63	ILE	3.7
2	D	24	ASP	3.7
2	E	22	ASP	3.6
2	F	59	GLY	3.6
1	C	545	THR	3.6
1	C	513	TRP	3.6
1	A	445	ARG	3.6
2	D	22	ASP	3.6
1	B	775	LEU	3.5
2	D	78	ASP	3.5
2	F	21	LYS	3.5
2	D	56	ASP	3.5
2	E	51	MET	3.4
1	C	740	GLN	3.4
1	C	767	GLN	3.4
2	F	37	ARG	3.4
2	D	61	GLY	3.4
2	E	58	ASP	3.4
2	E	34	THR	3.4
2	F	13	LYS	3.3
1	C	787	THR	3.3
2	D	49	GLN	3.3
1	A	798	ASP	3.3
1	B	797	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	52	ILE	3.3
2	E	147	ALA	3.3
1	C	739	LYS	3.3
2	D	68	PHE	3.2
2	D	43	PRO	3.2
1	B	774	LYS	3.2
2	E	57	ALA	3.2
1	C	518	ASN	3.2
2	E	79	THR	3.2
1	C	692	GLU	3.2
1	C	544	SER	3.2
2	E	74	ARG	3.1
1	C	786	GLU	3.1
2	E	24	ASP	3.1
2	F	121	VAL	3.1
2	E	75	LYS	3.0
1	B	768	LYS	3.0
2	F	106	ARG	3.0
1	C	672	ARG	3.0
2	D	9	ILE	3.0
2	E	116	LEU	2.9
2	E	56	ASP	2.9
2	D	51	MET	2.9
1	B	711	ILE	2.9
2	F	44	THR	2.9
1	B	785	ASN	2.9
1	A	741	ILE	2.9
1	B	426	ILE	2.9
1	C	785	ASN	2.9
2	F	61	GLY	2.8
1	B	702	SER	2.8
1	B	704	TYR	2.8
1	A	740	GLN	2.8
1	C	566	TYR	2.8
2	E	12	PHE	2.7
2	F	80	ASP	2.7
1	A	292	ARG	2.6
1	A	784	GLU	2.6
2	E	48	LEU	2.6
2	D	60	ASN	2.6
2	E	78	ASP	2.6
2	F	27	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	729	TYR	2.6
1	B	734	ASN	2.6
1	C	690	LYS	2.6
1	B	524	GLU	2.5
1	C	794	GLN	2.5
1	C	510	GLN	2.5
2	D	38	SER	2.5
2	F	17	SER	2.5
2	D	13	LYS	2.5
1	A	423	LYS	2.4
1	C	784	GLU	2.4
2	D	114	GLU	2.4
2	F	116	LEU	2.4
1	B	723	PHE	2.4
1	C	674	SER	2.4
2	E	67	GLU	2.4
1	C	499	PRO	2.4
2	D	72	MET	2.4
2	E	42	ASN	2.3
2	F	74	ARG	2.3
1	A	776	LEU	2.3
1	B	784	GLU	2.3
1	B	656	THR	2.3
2	F	6	GLU	2.3
2	E	7	GLU	2.3
1	A	659	THR	2.3
2	F	64	ASP	2.3
2	E	102	ALA	2.3
2	D	31	GLU	2.3
2	D	40	GLY	2.3
1	C	521	ASN	2.3
2	E	29	THR	2.3
1	B	793	PHE	2.3
2	D	15	ALA	2.2
2	E	115	LYS	2.2
1	B	715	GLU	2.2
1	B	743	PRO	2.2
2	D	12	PHE	2.2
2	E	65	PHE	2.2
1	C	729	TYR	2.2
2	F	53	ASN	2.2
2	E	73	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	787	THR	2.2
2	E	44	THR	2.2
2	D	74	ARG	2.2
1	C	691	LYS	2.1
2	E	27	ILE	2.1
2	D	62	THR	2.1
2	E	26	THR	2.1
1	B	763	LEU	2.1
2	E	20	ASP	2.1
2	F	24	ASP	2.1
2	F	50	ASP	2.1
1	A	712	PHE	2.1
1	B	751	TYR	2.1
1	B	786	GLU	2.1
1	B	742	ALA	2.1
1	C	430	LYS	2.1
2	D	80	ASP	2.0
2	D	73	ALA	2.0
1	C	517	VAL	2.0
1	C	773	PHE	2.0
1	B	750	GLN	2.0
1	B	788	ASP	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( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	1003	5/5	0.96	0.25	1.16	51,51,55,56	0
3	SO4	A	1001	5/5	0.98	0.23	0.47	42,42,44,47	0
4	CA	D	801	1/1	0.97	0.22	-0.58	57,57,57,57	0
4	CA	F	805	1/1	0.97	0.14	-1.07	66,66,66,66	0
4	CA	E	804	1/1	0.96	0.06	-1.60	81,81,81,81	0
4	CA	E	803	1/1	0.96	0.08	-1.98	79,79,79,79	0
4	CA	D	802	1/1	0.92	0.09	-2.77	61,61,61,61	0
4	CA	F	806	1/1	0.97	0.06	-3.10	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.