



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LMM  
Title : Crystal Structure of the DIP2311 protein from Corynebacterium diphtheriae, Northeast Structural Genomics Consortium Target CdR35  
Authors : Forouhar, F.; Lew, S.; Seetharaman, J.; Mao, M.; Xiao, R.; Ciccocanti, C.; Buchwald, W.A.; Maglaqui, M.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2010-01-31  
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

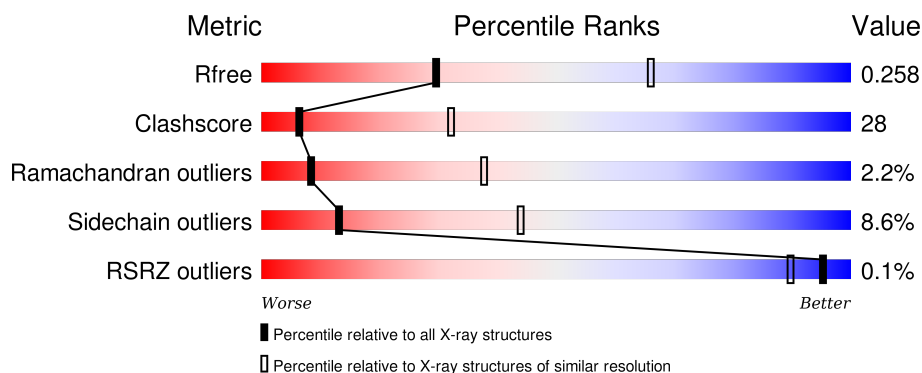
# 1 Overall quality at a glance

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	583	
1	B	583	
1	C	583	
1	D	583	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16408 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	Se	0	0	0
			3798	2390	682	716	4	6			
1	B	555	Total	C	N	O	S	Se	0	0	0
			4262	2673	766	808	6	9			
1	C	477	Total	C	N	O	S	Se	0	0	0
			3676	2312	659	695	4	6			
1	D	556	Total	C	N	O	S	Se	0	0	0
			4271	2678	767	811	6	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	EXPRESSION TAG	UNP Q6NEG3
A	576	LEU	-	EXPRESSION TAG	UNP Q6NEG3
A	577	GLU	-	EXPRESSION TAG	UNP Q6NEG3
A	578	HIS	-	EXPRESSION TAG	UNP Q6NEG3
A	579	HIS	-	EXPRESSION TAG	UNP Q6NEG3
A	580	HIS	-	EXPRESSION TAG	UNP Q6NEG3
A	581	HIS	-	EXPRESSION TAG	UNP Q6NEG3
A	582	HIS	-	EXPRESSION TAG	UNP Q6NEG3
A	583	HIS	-	EXPRESSION TAG	UNP Q6NEG3
B	1	VAL	-	EXPRESSION TAG	UNP Q6NEG3
B	576	LEU	-	EXPRESSION TAG	UNP Q6NEG3
B	577	GLU	-	EXPRESSION TAG	UNP Q6NEG3
B	578	HIS	-	EXPRESSION TAG	UNP Q6NEG3
B	579	HIS	-	EXPRESSION TAG	UNP Q6NEG3
B	580	HIS	-	EXPRESSION TAG	UNP Q6NEG3
B	581	HIS	-	EXPRESSION TAG	UNP Q6NEG3
B	582	HIS	-	EXPRESSION TAG	UNP Q6NEG3
B	583	HIS	-	EXPRESSION TAG	UNP Q6NEG3
C	1	VAL	-	EXPRESSION TAG	UNP Q6NEG3
C	576	LEU	-	EXPRESSION TAG	UNP Q6NEG3
C	577	GLU	-	EXPRESSION TAG	UNP Q6NEG3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	578	HIS	-	EXPRESSION TAG	UNP Q6NEG3
C	579	HIS	-	EXPRESSION TAG	UNP Q6NEG3
C	580	HIS	-	EXPRESSION TAG	UNP Q6NEG3
C	581	HIS	-	EXPRESSION TAG	UNP Q6NEG3
C	582	HIS	-	EXPRESSION TAG	UNP Q6NEG3
C	583	HIS	-	EXPRESSION TAG	UNP Q6NEG3
D	1	VAL	-	EXPRESSION TAG	UNP Q6NEG3
D	576	LEU	-	EXPRESSION TAG	UNP Q6NEG3
D	577	GLU	-	EXPRESSION TAG	UNP Q6NEG3
D	578	HIS	-	EXPRESSION TAG	UNP Q6NEG3
D	579	HIS	-	EXPRESSION TAG	UNP Q6NEG3
D	580	HIS	-	EXPRESSION TAG	UNP Q6NEG3
D	581	HIS	-	EXPRESSION TAG	UNP Q6NEG3
D	582	HIS	-	EXPRESSION TAG	UNP Q6NEG3
D	583	HIS	-	EXPRESSION TAG	UNP Q6NEG3

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Co 1 1	0	0
2	A	1	Total Co 1 1	0	0
2	D	1	Total Co 1 1	0	0
2	C	1	Total Co 1 1	0	0

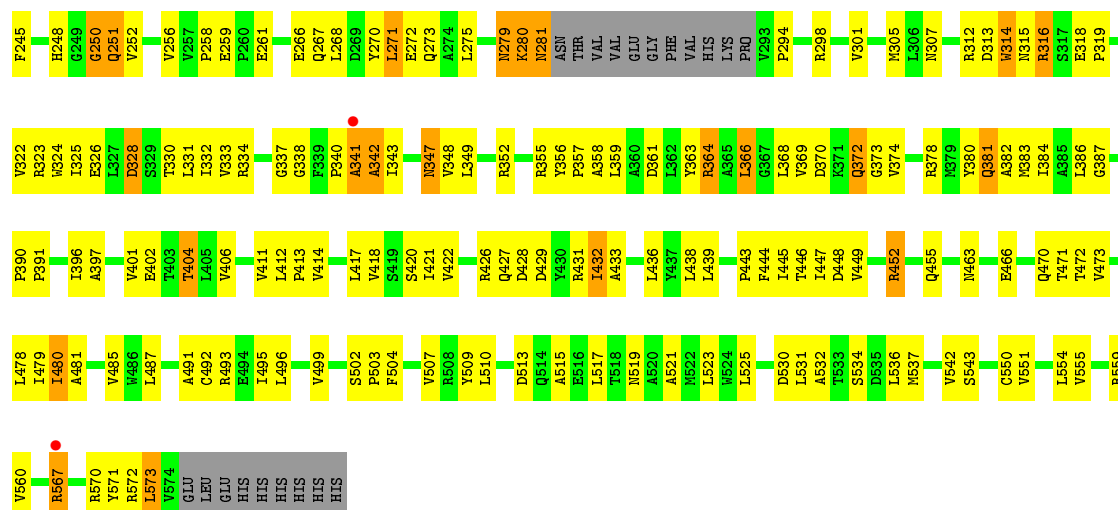
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	3	Total Cl 3 3	0	0
3	D	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

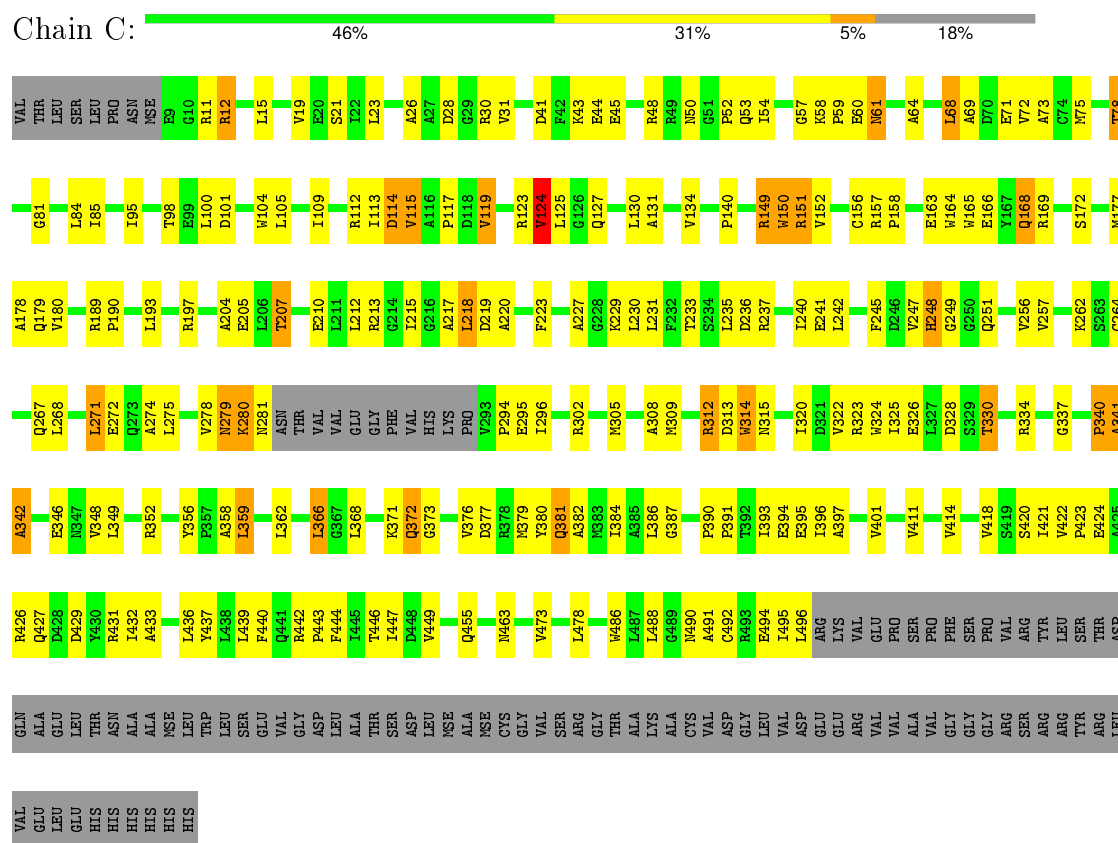
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total 128	O 128	0	0
4	B	64	Total 64	O 64	0	0
4	C	109	Total 109	O 109	0	0
4	D	90	Total 90	O 90	0	0

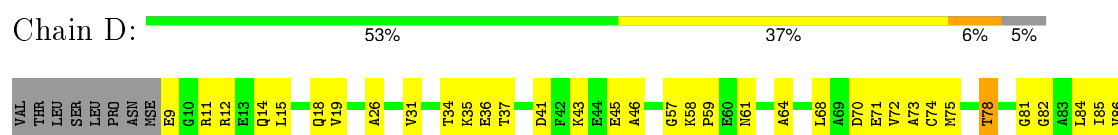




- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



E516	L517	T518	N519	M522	L525	S526	E527	D530	L531	S534	D535	L536	M537	A538	M539	G540	G541	V551	L554	V560	R567	S568	R569	R570	Y571	R572	L573	Y574	E575	LEU	GLU	HIS	HIS	HIS	HIS	HIS															
S420	I421	V422	P423	E424	R425	R426	Q427	I432	L436	R442	P443	F444	I445	T446	T447	D448	V449	Q455	E459	E466	V472	V473	L478	W486	L487	L488	Q490	A491	Q492	R493	E494	L495	L496	R497	R498	V499	S502	P503	F504	S505	V506	V507	R508	Y509	D513	Q514	A515				
A342	I343	T344	S345	E346	N347	V348	R352	R355	Y356	P357	A358	L359	D361	L362	Y363	L366	G367	L368	V369	Q372	G373	V376	M379	L380	Q381	A382	M383	I384	G387	P390	P391	T392	I393	E394	E395	I396	A397	F400	V401	E402	T403	T404	V411	L412	P413	V414	L417				
L271	E272	Q273	A274	L275	V278	N279	K280	N281	ASN	THR	VAL	VAL	GLU	PHE	VAL	HIS	LYS	PRO	V293	P294	E295	I296	R302	E303	A304	N307	A308	N309	R312	D313	R314	E318	P319	T320	D321	V322	R323	R324	I325	D328	S329	T330	L331	I332	V333	R334	G337	P340	A341		
W164	W165	E166	Y167	Q168	M177	R189	L193	K198	W199	L206	T207	D208	P209	E210	L218	D219	G222	P223	Q226	A227	G228	K229	T233	S234	L235	G126	Q127	D236	R237	I240	E241	L242	P245	G250	Q251	V252	V256	V257	P258	E259	P260	E261	E266	Q267	L268	D269	Y270				
W187	I188	E189	D190	K191	T192	R193	A194	I195	T198	E199	L100	D101	I102	D103	W104	L105	R106	Q107	G108	I109	F110	T111	I112	I113	D114	V115	A116	V119	V124	L125	G126	Q127	V134	P140	D143	D146	R147	L148	R149	W150	R151	V152	G153	C156	R157	P158	V159	D160	R161	A162	E163



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.31Å 102.03Å 164.51Å 90.00° 116.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 29.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.4 (19.99-3.00) 96.8 (29.93-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2 & XtalView	Depositor
R, $R_{free}$	0.183 , 0.231 0.208 , 0.258	Depositor DCC
$R_{free}$ test set	4106 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 6.6	EDS
Estimated twinning fraction	0.056 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 171986 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO, CL

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	0.41	0/3860	0.62	1/5239 (0.0%)
1	B	0.37	0/4325	0.58	0/5862
1	C	0.40	0/3734	0.60	0/5067
1	D	0.36	0/4334	0.57	0/5874
All	All	0.39	0/16253	0.59	1/22042 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	HIS	CB-CA-C	-6.45	97.49	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3798	0	3826	221	0
1	B	4262	0	4290	257	0
1	C	3676	0	3699	196	0
1	D	4271	0	4296	227	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	128	0	0	11	0
4	B	64	0	0	3	0
4	C	109	0	0	9	0
4	D	90	0	0	5	0
All	All	16408	0	16111	885	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 28.

All (885) 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:446:THR:HG22	1:B:449:VAL:HG23	1.19	1.19
1:C:271:LEU:HD12	1:C:305:MSE:HE1	1.32	1.10
1:D:446:THR:HG22	1:D:449:VAL:HG23	1.32	1.07
1:C:78:THR:HG23	1:C:150:TRP:HB2	1.42	1.01
1:B:177:MSE:HG2	1:B:359:LEU:HB2	1.51	0.93
1:B:470:GLN:HE22	1:D:57:GLY:H	1.08	0.93
1:C:387:GLY:HA3	1:C:411:VAL:HG22	1.48	0.93
1:A:446:THR:HG23	1:A:449:VAL:HG23	1.53	0.91
1:B:534:SER:HA	1:B:537:MSE:HE2	1.52	0.90
1:C:312:ARG:HH11	1:C:314:TRP:H	1.15	0.90
1:A:296:ILE:HG22	1:A:407:GLY:HA3	1.52	0.90
1:C:177:MSE:HG2	1:C:359:LEU:HB2	1.52	0.90
1:C:215:ILE:HD12	1:C:362:LEU:HD11	1.55	0.89
1:D:18:GLN:HE21	1:D:37:THR:HA	1.37	0.89
1:A:78:THR:HG21	1:A:151:ARG:HB2	1.56	0.88
1:B:422:VAL:HB	1:B:472:THR:HG23	1.56	0.88
1:A:151:ARG:HA	1:A:156:CYS:HB3	1.55	0.87
1:D:150:TRP:CE2	1:D:159:VAL:HG11	2.11	0.86
1:C:432:ILE:HD12	1:C:433:ALA:N	1.91	0.86
1:C:446:THR:HG22	1:C:449:VAL:HG23	1.58	0.85
1:A:246:ASP:HB3	4:A:599:HOH:O	1.76	0.84
1:C:312:ARG:HG2	1:C:313:ASP:H	1.42	0.84
1:B:108:GLY:O	1:B:112:ARG:HD2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASN:HA	1:A:294:PRO:HA	1.60	0.83
1:A:206:LEU:HB2	1:A:210:GLU:HG3	1.59	0.83
1:A:234:SER:HB3	1:A:261:GLU:O	1.78	0.82
1:B:472:THR:HG22	1:D:127:GLN:HE21	1.42	0.82
1:D:108:GLY:O	1:D:112:ARG:HD2	1.78	0.82
1:D:268:LEU:HB2	1:D:309:MSE:HE3	1.62	0.82
1:D:78:THR:HG21	1:D:151:ARG:HB2	1.60	0.82
1:C:248:HIS:HB2	4:C:653:HOH:O	1.80	0.81
1:B:109:ILE:O	1:B:113:ILE:HG22	1.79	0.81
1:A:70:ASP:OD2	1:A:143:ASP:HB2	1.81	0.81
1:D:421:ILE:HB	1:D:427:GLN:HG2	1.63	0.80
1:D:241:GLU:HB2	1:D:257:VAL:HG12	1.64	0.80
1:D:280:LYS:O	1:D:281:ASN:HB3	1.82	0.80
1:A:177:MSE:HG3	1:A:227:ALA:HB2	1.63	0.80
1:C:411:VAL:HG23	1:C:414:VAL:HB	1.64	0.80
1:B:436:LEU:HD21	1:B:478:LEU:HD22	1.62	0.80
1:C:151:ARG:HA	1:C:156:CYS:HB3	1.65	0.79
1:A:113:ILE:HG23	1:A:115:VAL:HG13	1.61	0.79
1:D:206:LEU:HB2	1:D:210:GLU:HG3	1.63	0.79
1:B:177:MSE:HG3	1:B:227:ALA:HB2	1.65	0.78
1:D:18:GLN:HG2	1:D:37:THR:HG22	1.66	0.78
1:A:150:TRP:CE2	1:A:159:VAL:HG11	2.19	0.77
1:B:332:ILE:HG12	1:B:404:THR:HG22	1.66	0.77
1:B:41:ASP:HB3	1:B:84:LEU:HG	1.67	0.77
1:C:95:ILE:HG12	1:C:124:VAL:HG21	1.67	0.76
1:D:11:ARG:HH21	1:D:14:GLN:HE21	1.30	0.76
1:D:152:VAL:HG21	1:D:157:ARG:HE	1.51	0.76
1:B:532:ALA:HB2	1:B:570:ARG:HE	1.51	0.76
1:B:85:ILE:HG22	1:B:88:ILE:HD13	1.68	0.76
1:A:109:ILE:O	1:A:113:ILE:HG22	1.85	0.75
1:B:312:ARG:HH11	1:B:314:TRP:H	1.33	0.75
1:B:78:THR:HG21	1:B:151:ARG:HB2	1.67	0.75
1:B:444:PHE:HB2	1:B:485:VAL:HG11	1.67	0.75
1:C:113:ILE:HG23	1:C:115:VAL:HG13	1.67	0.75
1:A:387:GLY:HA3	1:A:411:VAL:CG1	2.16	0.75
1:D:151:ARG:HA	1:D:156:CYS:HB3	1.69	0.75
1:B:151:ARG:HA	1:B:156:CYS:HB3	1.70	0.74
1:C:240:ILE:HG13	1:C:320:ILE:HB	1.70	0.74
1:D:387:GLY:HA3	1:D:411:VAL:HG12	1.68	0.74
1:B:420:SER:HB2	1:B:473:VAL:HG23	1.70	0.74
1:C:61:ASN:HD22	1:C:61:ASN:C	1.90	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG13	1:A:414:VAL:HB	1.69	0.74
1:B:446:THR:HG22	1:B:449:VAL:CG2	2.11	0.74
1:B:68:LEU:O	1:B:72:VAL:HG23	1.88	0.73
1:B:95:ILE:HG12	1:B:124:VAL:HG21	1.70	0.73
1:B:312:ARG:HH11	1:B:312:ARG:HG2	1.54	0.73
1:C:420:SER:HB2	1:C:473:VAL:HG23	1.70	0.73
1:C:30:ARG:HA	1:C:95:ILE:HD12	1.70	0.73
1:B:348:VAL:H	1:B:455:GLN:HE22	1.36	0.73
1:D:348:VAL:HG11	1:D:393:ILE:HD13	1.69	0.72
1:B:206:LEU:HB2	1:B:210:GLU:HG3	1.71	0.72
1:A:95:ILE:HG12	1:A:124:VAL:HG21	1.69	0.72
1:A:177:MSE:HB3	1:A:358:ALA:HB3	1.71	0.72
1:B:502:SER:HB2	1:B:503:PRO:HD2	1.70	0.72
1:D:98:THR:HG22	1:D:100:LEU:H	1.53	0.72
1:D:109:ILE:O	1:D:113:ILE:HG22	1.90	0.72
1:D:534:SER:HA	1:D:537:MSE:HE2	1.73	0.71
1:B:387:GLY:HA3	1:B:411:VAL:HG12	1.72	0.71
1:D:502:SER:HB3	1:D:503:PRO:HD2	1.71	0.71
1:A:177:MSE:HG2	1:A:359:LEU:HB2	1.73	0.71
1:A:100:LEU:O	1:A:128:ARG:NH1	2.24	0.71
1:A:242:LEU:HB3	1:A:256:VAL:HG13	1.71	0.70
1:B:281:ASN:HA	1:B:294:PRO:HA	1.72	0.70
1:A:26:ALA:HB1	1:A:125:LEU:HD11	1.74	0.70
1:D:75:MSE:HE2	1:D:81:GLY:O	1.91	0.70
1:A:312:ARG:HD3	1:A:314:TRP:CD2	2.27	0.70
1:C:109:ILE:O	1:C:113:ILE:HG22	1.92	0.70
1:D:271:LEU:HD12	1:D:305:MSE:HE1	1.75	0.69
1:B:271:LEU:HB3	1:B:305:MSE:HE1	1.73	0.69
1:B:387:GLY:HA3	1:B:411:VAL:CG1	2.23	0.69
1:A:149:ARG:HB3	1:A:158:PRO:HA	1.75	0.69
1:C:312:ARG:HG2	1:C:313:ASP:N	2.06	0.69
1:D:74:CYS:O	1:D:78:THR:HG22	1.93	0.69
1:B:73:ALA:HB2	1:B:113:ILE:HD11	1.75	0.69
1:A:312:ARG:HG2	1:A:312:ARG:HH11	1.58	0.69
1:A:332:ILE:HG23	1:A:404:THR:HG23	1.73	0.69
1:B:235:LEU:HD21	1:B:267:GLN:NE2	2.09	0.68
1:B:150:TRP:CE2	1:B:159:VAL:HG11	2.27	0.68
1:C:41:ASP:HB3	1:C:84:LEU:HG	1.74	0.68
1:D:177:MSE:HG3	1:D:227:ALA:HB2	1.76	0.68
1:C:312:ARG:HD3	1:C:314:TRP:CD2	2.28	0.68
1:C:492:CYS:O	1:C:496:LEU:HD13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG21	1:A:157:ARG:HD3	1.75	0.68
1:B:480:ILE:HD13	1:B:481:ALA:H	1.59	0.68
1:B:444:PHE:HB2	1:B:485:VAL:CG1	2.24	0.68
1:B:480:ILE:HD13	1:B:481:ALA:N	2.08	0.68
1:A:229:LYS:O	1:A:233:THR:HB	1.94	0.68
1:A:312:ARG:HH11	1:A:314:TRP:H	1.39	0.68
1:C:312:ARG:NH1	1:C:314:TRP:H	1.90	0.67
1:C:229:LYS:O	1:C:233:THR:HB	1.95	0.67
1:D:26:ALA:HB1	1:D:125:LEU:HD21	1.75	0.67
1:C:98:THR:HG22	1:C:100:LEU:H	1.59	0.67
1:B:492:CYS:O	1:B:496:LEU:HD23	1.95	0.67
1:B:432:ILE:C	1:B:432:ILE:HD12	2.15	0.67
1:C:366:LEU:HB3	1:C:368:LEU:HD13	1.77	0.67
1:B:417:LEU:HD21	1:B:492:CYS:SG	2.35	0.66
1:B:348:VAL:H	1:B:455:GLN:NE2	1.93	0.66
1:D:312:ARG:HH11	1:D:314:TRP:H	1.41	0.66
1:C:346:GLU:HA	1:C:455:GLN:HE22	1.60	0.66
1:D:125:LEU:HD22	1:D:125:LEU:H	1.61	0.66
1:D:413:PRO:CG	1:D:499:VAL:HG22	2.25	0.66
1:D:177:MSE:HG2	1:D:359:LEU:HB2	1.75	0.66
1:D:334:ARG:HG2	1:D:400:PHE:CD1	2.31	0.66
1:D:387:GLY:HA3	1:D:411:VAL:CG1	2.26	0.66
1:D:411:VAL:HG13	1:D:414:VAL:HB	1.77	0.66
1:A:242:LEU:HB3	1:A:256:VAL:CG1	2.26	0.66
1:B:235:LEU:H	1:B:235:LEU:HD23	1.59	0.66
1:C:387:GLY:HA3	1:C:411:VAL:CG2	2.25	0.66
1:B:64:ALA:O	1:B:68:LEU:HD23	1.95	0.66
1:B:92:THR:OG1	1:B:94:ARG:HG2	1.96	0.66
1:B:219:ASP:HB2	1:B:223:PHE:O	1.95	0.66
1:B:177:MSE:HB3	1:B:358:ALA:HB3	1.78	0.66
1:D:11:ARG:NH2	1:D:14:GLN:HE21	1.93	0.66
1:B:30:ARG:HA	1:B:95:ILE:HD12	1.79	0.65
1:A:26:ALA:HB1	1:A:125:LEU:CD1	2.26	0.65
1:C:140:PRO:HD3	1:C:164:TRP:CZ3	2.31	0.65
1:A:424:GLU:O	1:A:427:GLN:HG3	1.96	0.65
1:A:381:GLN:HG3	1:A:382:ALA:N	2.11	0.65
1:C:394:GLU:HG2	1:C:395:GLU:N	2.12	0.65
1:A:387:GLY:HA3	1:A:411:VAL:HG12	1.78	0.65
1:C:380:TYR:CE2	1:C:391:PRO:HG2	2.31	0.65
1:C:219:ASP:HB3	1:C:223:PHE:H	1.61	0.65
1:D:235:LEU:H	1:D:235:LEU:HD23	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:VAL:HG11	1:B:492:CYS:SG	2.38	0.64
1:B:98:THR:HG22	1:B:100:LEU:H	1.63	0.64
1:B:49:ARG:HD3	1:B:54:ILE:HG22	1.80	0.64
1:B:19:VAL:HG13	1:B:85:ILE:HD11	1.80	0.64
1:A:344:THR:HG23	1:A:346:GLU:H	1.62	0.64
1:D:140:PRO:HG2	1:D:361:ASP:OD1	1.97	0.64
1:D:177:MSE:HB3	1:D:358:ALA:HB3	1.79	0.63
1:B:426:ARG:HG2	1:B:426:ARG:HH21	1.62	0.63
1:B:235:LEU:HD21	1:B:267:GLN:HE22	1.63	0.63
1:D:68:LEU:O	1:D:72:VAL:HG23	1.98	0.63
1:A:95:ILE:HD13	1:A:125:LEU:HD13	1.79	0.63
1:D:140:PRO:HD3	1:D:164:TRP:CZ3	2.33	0.63
1:A:354:ALA:HB1	4:A:673:HOH:O	1.99	0.63
1:D:102:ILE:HG23	1:D:119:VAL:HG13	1.81	0.63
1:D:341:ALA:O	1:D:342:ALA:HB2	1.99	0.63
1:C:280:LYS:HZ3	1:C:326:GLU:CB	2.12	0.63
1:A:151:ARG:NE	4:A:606:HOH:O	2.32	0.63
1:D:151:ARG:HB3	1:D:151:ARG:HH11	1.63	0.63
1:A:379:MSE:HE3	1:A:391:PRO:CG	2.29	0.62
1:D:279:ASN:HD21	1:D:296:ILE:H	1.46	0.62
1:C:414:VAL:O	1:C:418:VAL:HG23	1.99	0.62
1:C:68:LEU:O	1:C:72:VAL:HG23	1.98	0.62
1:B:444:PHE:HE1	1:B:523:LEU:HB3	1.64	0.62
1:C:443:PRO:HG2	1:C:444:PHE:HD1	1.64	0.62
1:A:496:LEU:O	1:A:499:VAL:HG23	1.99	0.62
1:C:432:ILE:C	1:C:432:ILE:HD12	2.19	0.62
1:C:421:ILE:HB	1:C:427:GLN:HG2	1.81	0.62
1:A:423:PRO:HG3	1:C:54:ILE:HD11	1.81	0.62
1:A:235:LEU:HD21	1:A:267:GLN:HE22	1.63	0.62
1:C:235:LEU:HD21	1:C:267:GLN:NE2	2.15	0.62
1:C:58:LYS:HE3	4:C:647:HOH:O	2.00	0.62
1:B:12:ARG:O	1:B:16:ILE:HG13	1.98	0.62
1:A:344:THR:HG22	1:A:347:ASN:HB2	1.80	0.62
1:C:382:ALA:O	1:C:386:LEU:HD13	2.00	0.62
1:D:275:LEU:HD22	1:D:305:MSE:HE2	1.82	0.61
1:A:271:LEU:HD12	1:A:305:MSE:HE1	1.83	0.61
1:A:432:ILE:HD12	1:A:432:ILE:C	2.20	0.61
1:A:163:GLU:HG3	1:B:163:GLU:HG3	1.82	0.61
1:D:328:ASP:HB3	1:D:330:THR:HG23	1.81	0.61
1:A:86:VAL:HG12	1:A:98:THR:HG21	1.81	0.61
1:A:200:ASP:HB3	1:A:203:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:THR:CG2	1:B:449:VAL:HG23	2.12	0.61
1:C:280:LYS:HZ3	1:C:326:GLU:HB3	1.64	0.61
1:C:54:ILE:HG13	1:C:54:ILE:O	2.00	0.61
1:B:352:ARG:CZ	1:B:373:GLY:HA3	2.31	0.61
1:C:60:GLU:HG2	1:C:104:TRP:CD1	2.35	0.61
1:C:178:ALA:HB2	1:C:358:ALA:HB2	1.82	0.61
1:D:31:VAL:HG13	1:D:95:ILE:HD11	1.81	0.61
1:B:470:GLN:NE2	1:D:57:GLY:H	1.90	0.61
1:A:160:ASP:OD1	1:A:162:ALA:HB3	2.01	0.61
1:B:550:CYS:O	1:B:554:LEU:HD13	2.00	0.61
1:D:177:MSE:HE3	1:D:359:LEU:HG	1.83	0.60
1:B:242:LEU:HB3	1:B:256:VAL:HG13	1.84	0.60
1:D:68:LEU:HD21	1:D:86:VAL:HG11	1.83	0.60
1:C:381:GLN:HG3	1:C:382:ALA:N	2.17	0.60
1:B:325:ILE:HG21	1:B:328:ASP:OD2	2.02	0.60
1:B:140:PRO:HD3	1:B:164:TRP:CZ3	2.36	0.60
1:C:280:LYS:O	1:C:281:ASN:HB3	2.02	0.60
1:D:344:THR:HG22	1:D:347:ASN:HD22	1.66	0.60
1:A:383:MSE:HG3	1:A:391:PRO:HD3	1.83	0.60
1:C:280:LYS:HE3	1:C:295:GLU:OE1	2.02	0.59
1:D:503:PRO:HA	1:D:508:ARG:NH1	2.17	0.59
1:B:109:ILE:HG22	1:B:113:ILE:HG21	1.85	0.59
1:A:73:ALA:HB2	1:A:113:ILE:HD11	1.85	0.59
1:A:165:TRP:CE3	1:A:168:GLN:HG2	2.38	0.59
1:A:472:THR:HG21	1:C:125:LEU:O	2.03	0.59
1:A:108:GLY:O	1:A:112:ARG:HD2	2.03	0.59
1:B:312:ARG:NH1	1:B:314:TRP:H	2.01	0.59
1:D:219:ASP:HB2	1:D:223:PHE:O	2.03	0.59
1:D:43:LYS:HE3	1:D:71:GLU:CD	2.23	0.59
1:C:31:VAL:HG13	1:C:95:ILE:HD11	1.85	0.59
1:D:499:VAL:HG11	1:D:506:PRO:HD2	1.84	0.58
1:A:316:ARG:HG2	1:A:316:ARG:HH11	1.68	0.58
1:C:242:LEU:HB3	1:C:256:VAL:HG13	1.85	0.58
1:D:424:GLU:O	1:D:427:GLN:HG3	2.02	0.58
1:B:242:LEU:HB2	1:B:271:LEU:HD11	1.84	0.58
1:A:492:CYS:O	1:A:496:LEU:HD23	2.03	0.58
1:A:446:THR:CG2	1:A:449:VAL:HG23	2.30	0.58
1:D:124:VAL:HB	1:D:125:LEU:HD22	1.85	0.58
1:D:235:LEU:HD21	1:D:267:GLN:HE22	1.67	0.58
1:A:416:GLU:HA	1:A:419:SER:HB3	1.84	0.58
1:B:149:ARG:HB3	1:B:158:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:LEU:HD21	1:C:478:LEU:HD22	1.85	0.58
1:B:275:LEU:HD21	1:B:331:LEU:HD11	1.85	0.58
1:A:43:LYS:HD2	1:A:71:GLU:HG2	1.85	0.58
1:B:530:ASP:OD1	1:B:572:ARG:HB2	2.03	0.58
1:B:411:VAL:HG13	1:B:414:VAL:HB	1.86	0.58
1:B:9:GLU:CD	1:B:10:GLY:H	2.06	0.58
1:A:78:THR:CG2	1:A:151:ARG:H	2.15	0.58
1:B:426:ARG:HD3	1:B:471:THR:OG1	2.04	0.58
1:C:446:THR:CG2	1:C:449:VAL:HG23	2.33	0.58
1:D:432:ILE:HD12	1:D:432:ILE:C	2.24	0.58
1:A:316:ARG:HG2	1:A:316:ARG:NH1	2.17	0.57
1:B:525:LEU:HD21	1:B:531:LEU:HB3	1.86	0.57
1:A:150:TRP:CZ2	1:A:159:VAL:HG11	2.38	0.57
1:D:413:PRO:HG3	1:D:499:VAL:HG22	1.85	0.57
1:A:362:LEU:O	1:A:366:LEU:HD23	2.03	0.57
1:A:124:VAL:HG23	1:A:125:LEU:N	2.19	0.57
1:B:560:VAL:HA	1:B:573:LEU:HA	1.87	0.57
1:A:355:ARG:HD2	1:A:356:TYR:CE2	2.39	0.57
1:D:189:ARG:HD3	1:D:266:GLU:OE1	2.04	0.57
1:B:23:LEU:HD22	1:B:124:VAL:CG1	2.35	0.57
1:D:161:ARG:HD3	1:D:361:ASP:OD2	2.04	0.57
1:D:396:ILE:HG22	1:D:397:ALA:N	2.20	0.57
1:D:312:ARG:NH1	1:D:314:TRP:H	2.03	0.57
1:B:352:ARG:NH1	1:B:373:GLY:HA3	2.19	0.57
1:C:177:MSE:HG3	1:C:227:ALA:HB2	1.86	0.57
1:B:443:PRO:HA	1:B:509:TYR:CE2	2.39	0.57
1:B:207:THR:OG1	1:B:210:GLU:HG2	2.03	0.57
1:A:316:ARG:CG	1:A:316:ARG:HH11	2.18	0.57
1:B:200:ASP:OD1	1:B:202:ALA:HB3	2.05	0.57
1:B:60:GLU:HG2	1:B:104:TRP:CE2	2.39	0.56
1:C:166:GLU:OE1	1:D:166:GLU:OE1	2.23	0.56
1:A:31:VAL:HG13	1:A:95:ILE:HD11	1.86	0.56
1:B:242:LEU:HB3	1:B:256:VAL:CG1	2.36	0.56
1:D:235:LEU:HD21	1:D:267:GLN:NE2	2.20	0.56
1:A:337:GLY:O	1:A:401:VAL:HG23	2.05	0.56
1:A:316:ARG:HH21	1:A:399:PRO:CD	2.19	0.56
1:B:102:ILE:HG23	1:B:119:VAL:HG13	1.86	0.56
1:C:272:GLU:OE2	1:C:302:ARG:HG3	2.06	0.56
1:A:68:LEU:HD21	1:A:86:VAL:HG21	1.88	0.56
1:A:150:TRP:NE1	1:A:159:VAL:HG11	2.20	0.56
1:B:496:LEU:O	1:B:499:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:HG2	1:A:426:ARG:HH21	1.70	0.56
1:C:309:MSE:HG3	4:C:600:HOH:O	2.05	0.56
1:B:160:ASP:OD1	1:B:162:ALA:HB3	2.06	0.56
1:A:61:ASN:HD22	1:A:61:ASN:C	2.08	0.56
1:D:207:THR:OG1	1:D:210:GLU:HG2	2.05	0.56
1:D:258:PRO:HB2	1:D:267:GLN:HG2	1.87	0.56
1:D:125:LEU:HD22	1:D:125:LEU:N	2.20	0.56
1:C:43:LYS:HE3	1:C:71:GLU:OE2	2.06	0.56
1:D:75:MSE:O	1:D:78:THR:HG23	2.05	0.55
1:A:207:THR:OG1	1:A:210:GLU:HG2	2.05	0.55
1:C:380:TYR:O	1:C:384:ILE:HG12	2.06	0.55
1:D:344:THR:H	1:D:347:ASN:HB2	1.71	0.55
1:A:189:ARG:HD3	1:A:266:GLU:OE1	2.07	0.55
1:C:61:ASN:ND2	1:C:61:ASN:C	2.56	0.55
1:A:312:ARG:HD3	1:A:314:TRP:CE3	2.40	0.55
1:D:394:GLU:HG2	1:D:395:GLU:N	2.21	0.55
1:D:417:LEU:HG	1:D:496:LEU:HD21	1.88	0.55
1:B:366:LEU:HB3	1:B:368:LEU:HD13	1.87	0.55
1:B:258:PRO:HB2	1:B:267:GLN:HG2	1.88	0.55
1:C:235:LEU:HD21	1:C:267:GLN:HE22	1.71	0.55
1:D:36:GLU:HG2	4:D:597:HOH:O	2.05	0.55
1:C:75:MSE:HE2	1:C:81:GLY:C	2.26	0.55
1:B:75:MSE:O	1:B:78:THR:HG23	2.07	0.55
1:D:245:PHE:HE1	1:D:252:VAL:HG22	1.72	0.55
1:D:443:PRO:HA	1:D:509:TYR:CZ	2.41	0.55
1:A:124:VAL:HG23	1:A:125:LEU:H	1.70	0.54
1:D:432:ILE:HD12	1:D:432:ILE:O	2.06	0.54
1:D:143:ASP:OD1	1:D:147:ARG:HG2	2.06	0.54
1:C:271:LEU:CD1	1:C:305:MSE:HE1	2.22	0.54
1:A:316:ARG:HH21	1:A:399:PRO:HD2	1.72	0.54
1:B:113:ILE:HG23	1:B:115:VAL:HG12	1.89	0.54
1:C:242:LEU:HB3	1:C:256:VAL:CG1	2.37	0.54
1:A:60:GLU:HG2	1:A:104:TRP:CD1	2.41	0.54
1:C:68:LEU:HD23	1:C:105:LEU:HD21	1.88	0.54
1:A:41:ASP:HB3	1:A:84:LEU:HG	1.89	0.54
1:C:177:MSE:HB3	1:C:358:ALA:HB3	1.89	0.54
1:C:433:ALA:HB2	4:C:598:HOH:O	2.07	0.54
1:C:384:ILE:HD11	1:C:390:PRO:HB3	1.90	0.54
1:C:217:ALA:HA	4:C:662:HOH:O	2.07	0.54
1:C:197:ARG:HH11	1:C:197:ARG:HG2	1.72	0.54
1:A:78:THR:HG22	1:A:151:ARG:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ARG:HH11	1:C:53:GLN:NE2	2.05	0.54
1:B:312:ARG:HG2	1:B:312:ARG:NH1	2.21	0.54
1:A:238:THR:HB	4:A:664:HOH:O	2.07	0.54
1:D:113:ILE:HG23	1:D:115:VAL:HG13	1.90	0.54
1:A:271:LEU:HB3	1:A:305:MSE:HE1	1.89	0.54
1:C:312:ARG:HH11	1:C:314:TRP:N	1.96	0.54
1:A:412:LEU:O	1:A:416:GLU:HG2	2.08	0.54
1:A:90:ASP:OD2	1:A:91:LYS:HG3	2.08	0.54
1:C:346:GLU:HA	1:C:455:GLN:NE2	2.22	0.53
1:C:115:VAL:HG22	1:C:117:PRO:HD3	1.90	0.53
1:A:341:ALA:O	1:A:342:ALA:HB2	2.07	0.53
1:A:331:LEU:HD21	1:A:333:VAL:HG23	1.90	0.53
1:D:95:ILE:HG13	1:D:125:LEU:HD23	1.89	0.53
1:A:113:ILE:O	1:A:114:ASP:HB2	2.09	0.53
1:B:150:TRP:CZ2	1:B:159:VAL:HG11	2.44	0.53
1:A:412:LEU:HD22	1:A:412:LEU:H	1.74	0.53
1:C:325:ILE:HB	1:C:330:THR:HG23	1.91	0.53
1:C:105:LEU:O	1:C:109:ILE:HG13	2.08	0.53
1:B:396:ILE:HG22	1:B:397:ALA:N	2.23	0.53
1:A:140:PRO:HD3	1:A:164:TRP:CZ3	2.44	0.53
1:D:64:ALA:O	1:D:68:LEU:HD13	2.08	0.53
1:D:303:GLU:O	1:D:307:ASN:HB2	2.08	0.53
1:D:45:GLU:OE2	1:D:98:THR:HG23	2.07	0.53
1:A:235:LEU:HD21	1:A:267:GLN:NE2	2.24	0.53
1:C:219:ASP:OD2	1:C:220:ALA:N	2.42	0.52
1:C:124:VAL:HG23	1:C:125:LEU:H	1.75	0.52
1:B:165:TRP:O	1:B:169:ARG:HG3	2.09	0.52
1:A:75:MSE:HG2	1:A:134:VAL:HG13	1.91	0.52
1:B:26:ALA:HB1	1:B:125:LEU:CD2	2.40	0.52
1:C:341:ALA:O	1:C:342:ALA:HB2	2.09	0.52
1:C:213:ARG:NH1	1:C:218:LEU:HD12	2.25	0.52
1:D:90:ASP:O	1:D:91:LYS:HB2	2.09	0.52
1:A:78:THR:HG22	1:A:150:TRP:HB2	1.92	0.52
1:D:75:MSE:HG2	1:D:134:VAL:HG13	1.91	0.52
1:B:438:LEU:HB3	1:B:445:ILE:HD13	1.90	0.52
1:B:536:LEU:O	1:B:536:LEU:HD13	2.10	0.52
1:A:240:ILE:HG13	1:A:320:ILE:HB	1.90	0.52
1:C:69:ALA:O	1:C:113:ILE:HD12	2.10	0.52
1:A:379:MSE:HE3	1:A:391:PRO:HG3	1.91	0.52
1:D:34:THR:HG22	1:D:37:THR:OG1	2.10	0.52
1:B:519:ASN:ND2	1:B:523:LEU:HD13	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HD12	1:B:211:LEU:HA	1.91	0.52
1:B:22:ILE:HD11	1:B:40:VAL:HG21	1.91	0.52
1:B:197:ARG:HG2	1:B:197:ARG:HH11	1.74	0.52
1:D:446:THR:HG23	1:D:448:ASP:H	1.75	0.52
1:D:240:ILE:HG13	1:D:320:ILE:HB	1.92	0.52
1:C:23:LEU:HD22	1:C:124:VAL:CG1	2.40	0.52
1:C:190:PRO:HB2	4:C:634:HOH:O	2.09	0.52
1:C:241:GLU:HB2	1:C:257:VAL:HG12	1.90	0.52
1:C:113:ILE:CG2	1:C:115:VAL:HG13	2.39	0.51
1:B:420:SER:CB	1:B:473:VAL:HG23	2.39	0.51
1:C:11:ARG:HH21	1:C:11:ARG:HG3	1.75	0.51
1:A:85:ILE:HG22	1:A:88:ILE:HD13	1.92	0.51
1:C:50:ASN:O	1:C:52:PRO:HD2	2.09	0.51
1:A:313:ASP:C	1:A:315:ASN:H	2.14	0.51
1:B:245:PHE:HE1	1:B:252:VAL:HG22	1.75	0.51
1:D:333:VAL:O	1:D:402:GLU:HA	2.09	0.51
1:D:312:ARG:HH11	1:D:314:TRP:N	2.09	0.51
1:A:391:PRO:HA	4:A:614:HOH:O	2.09	0.51
1:D:325:ILE:HG21	1:D:328:ASP:HB2	1.92	0.51
1:D:229:LYS:O	1:D:233:THR:HB	2.10	0.51
1:B:30:ARG:HB3	1:B:94:ARG:HA	1.91	0.51
1:D:313:ASP:O	1:D:314:TRP:HB2	2.09	0.51
1:A:168:GLN:O	1:A:172:SER:HB2	2.11	0.51
1:A:54:ILE:HD12	1:A:55:GLU:O	2.10	0.51
1:C:274:ALA:O	1:C:278:VAL:HG23	2.11	0.51
1:B:298:ARG:HG3	1:B:298:ARG:HH21	1.76	0.51
1:C:396:ILE:HG22	1:C:397:ALA:N	2.24	0.51
1:A:280:LYS:O	1:A:281:ASN:HB3	2.09	0.51
1:A:439:LEU:HD13	1:A:488:LEU:HB2	1.93	0.51
1:C:312:ARG:HH11	1:C:312:ARG:HG2	1.75	0.51
1:C:328:ASP:O	1:C:330:THR:HG22	2.11	0.51
1:A:417:LEU:C	1:A:417:LEU:HD13	2.31	0.51
1:D:412:LEU:HD22	1:D:412:LEU:H	1.76	0.51
1:A:108:GLY:O	1:A:112:ARG:CD	2.59	0.51
1:D:92:THR:OG1	1:D:94:ARG:HG2	2.11	0.51
1:B:338:GLY:HA2	1:B:401:VAL:HG23	1.92	0.51
1:D:75:MSE:HE2	1:D:81:GLY:C	2.30	0.51
1:B:525:LEU:HB3	1:B:573:LEU:HG	1.93	0.51
1:C:149:ARG:HB3	1:C:158:PRO:HA	1.93	0.51
1:A:493:ARG:O	1:A:497:ARG:HG3	2.10	0.51
1:C:424:GLU:O	1:C:427:GLN:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:O	1:B:402:GLU:HA	2.11	0.50
1:B:341:ALA:O	1:B:342:ALA:HB2	2.11	0.50
1:A:480:ILE:HG22	1:A:487:LEU:HD12	1.94	0.50
1:D:411:VAL:HG22	1:D:413:PRO:HG2	1.93	0.50
1:A:23:LEU:HD22	1:A:124:VAL:CG1	2.42	0.50
1:A:61:ASN:ND2	1:A:61:ASN:C	2.65	0.50
1:A:443:PRO:HG2	1:A:444:PHE:HD1	1.76	0.50
1:D:513:ASP:OD2	1:D:515:ALA:HB3	2.11	0.50
1:C:23:LEU:HD22	1:C:124:VAL:HG13	1.94	0.50
1:B:496:LEU:HB3	1:B:507:VAL:HG21	1.94	0.50
1:B:145:SER:HB2	1:B:147:ARG:HG2	1.93	0.50
1:B:357:PRO:HD2	3:B:584:CL:CL	2.49	0.50
1:B:472:THR:HG22	1:D:127:GLN:NE2	2.18	0.50
1:D:113:ILE:HG23	1:D:115:VAL:CG1	2.42	0.50
1:D:193:LEU:HD13	1:D:208:ASP:CG	2.32	0.50
1:D:75:MSE:HE3	1:D:78:THR:HG23	1.94	0.50
1:D:275:LEU:HD22	1:D:305:MSE:CE	2.41	0.50
1:D:355:ARG:HD2	1:D:356:TYR:CE2	2.47	0.50
1:C:43:LYS:HD3	4:C:669:HOH:O	2.11	0.50
1:C:207:THR:OG1	1:C:210:GLU:HG3	2.11	0.50
1:A:328:ASP:HB3	1:A:330:THR:HG23	1.93	0.50
1:B:235:LEU:CD2	1:B:235:LEU:H	2.23	0.50
1:D:43:LYS:HE3	1:D:71:GLU:OE2	2.11	0.50
1:C:43:LYS:HE3	1:C:71:GLU:CD	2.33	0.50
1:B:340:PRO:O	1:B:342:ALA:N	2.45	0.50
1:D:75:MSE:HE3	1:D:78:THR:CG2	2.42	0.50
1:D:11:ARG:HH21	1:D:14:GLN:NE2	2.04	0.50
1:A:411:VAL:HG22	1:A:413:PRO:HG2	1.94	0.50
1:C:422:VAL:HA	1:C:423:PRO:C	2.31	0.50
1:C:376:VAL:HG13	1:C:377:ASP:N	2.27	0.50
1:A:50:ASN:O	1:A:52:PRO:HD2	2.12	0.50
1:D:560:VAL:HA	1:D:573:LEU:HA	1.94	0.50
1:C:446:THR:HG22	1:C:449:VAL:CG2	2.37	0.49
1:D:312:ARG:NH1	1:D:314:TRP:HA	2.27	0.49
1:D:531:LEU:HD23	1:D:531:LEU:C	2.32	0.49
1:A:490:ASN:O	1:A:494:GLU:HG2	2.12	0.49
1:A:75:MSE:HE3	1:A:75:MSE:HA	1.94	0.49
1:A:246:ASP:HB2	1:A:253:LEU:HD11	1.94	0.49
1:B:87:GLY:C	1:B:88:ILE:HD12	2.31	0.49
1:C:236:ASP:O	1:C:237:ARG:HB3	2.12	0.49
1:D:41:ASP:HB3	1:D:84:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LEU:HD12	1:C:305:MSE:CE	2.23	0.49
1:D:109:ILE:HG22	1:D:113:ILE:HG21	1.95	0.49
1:A:312:ARG:HG2	1:A:314:TRP:H	1.77	0.49
1:D:19:VAL:HG13	1:D:85:ILE:HD11	1.94	0.49
1:D:332:ILE:HG12	1:D:404:THR:HG22	1.94	0.49
1:D:383:MSE:HG3	1:D:391:PRO:HD3	1.94	0.49
1:C:95:ILE:HD13	1:C:125:LEU:HD23	1.93	0.49
1:C:109:ILE:HG22	1:C:113:ILE:CG2	2.43	0.49
1:B:413:PRO:CG	1:B:499:VAL:HG22	2.42	0.49
1:A:313:ASP:O	1:A:315:ASN:N	2.46	0.49
1:A:235:LEU:H	1:A:235:LEU:HD23	1.77	0.49
1:C:348:VAL:HG23	1:C:349:LEU:HD12	1.94	0.49
1:A:150:TRP:NE1	1:A:159:VAL:CG1	2.76	0.49
1:B:229:LYS:O	1:B:233:THR:HB	2.12	0.49
1:A:298:ARG:HD3	3:A:586:CL:CL	2.50	0.49
1:A:197:ARG:NH1	1:A:197:ARG:HG2	2.28	0.49
1:A:387:GLY:HA3	1:A:411:VAL:HG11	1.94	0.49
1:C:281:ASN:H	1:C:295:GLU:HG3	1.78	0.49
1:D:522:MSE:HE3	1:D:573:LEU:HD23	1.94	0.49
1:C:334:ARG:HG3	1:C:334:ARG:HH11	1.77	0.49
1:A:281:ASN:CA	1:A:294:PRO:HA	2.39	0.49
1:C:30:ARG:CA	1:C:95:ILE:HD12	2.42	0.49
1:B:330:THR:HG22	1:B:406:VAL:HA	1.94	0.49
1:C:394:GLU:HG2	1:C:395:GLU:H	1.77	0.49
1:B:384:ILE:HD11	1:B:390:PRO:HB3	1.93	0.49
1:B:452:ARG:NH2	1:B:452:ARG:HB2	2.28	0.49
1:A:102:ILE:HG23	1:A:119:VAL:HG13	1.95	0.49
1:D:198:LYS:HG3	1:D:199:TRP:N	2.28	0.49
1:B:177:MSE:O	1:B:226:GLN:HB3	2.12	0.49
1:B:242:LEU:HA	1:B:322:VAL:HG13	1.94	0.49
1:A:258:PRO:HB2	1:A:267:GLN:HG2	1.95	0.49
1:D:234:SER:HB3	1:D:261:GLU:O	2.12	0.49
1:C:426:ARG:HH21	1:C:426:ARG:HG3	1.78	0.49
1:B:355:ARG:HD2	1:B:356:TYR:CE2	2.48	0.49
1:B:74:CYS:O	1:B:78:THR:HG22	2.13	0.49
1:B:95:ILE:HD13	1:B:125:LEU:HD23	1.95	0.49
1:A:95:ILE:O	1:C:423:PRO:HB3	2.13	0.48
1:A:312:ARG:HH11	1:A:312:ARG:CG	2.26	0.48
1:C:193:LEU:HD21	1:C:212:LEU:HD21	1.95	0.48
1:D:384:ILE:HD11	1:D:390:PRO:HB3	1.94	0.48
1:A:185:LEU:HD13	1:A:209:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:ARG:HH21	1:D:426:ARG:HG2	1.78	0.48
1:B:491:ALA:O	1:B:495:ILE:HG12	2.13	0.48
1:D:340:PRO:O	1:D:342:ALA:N	2.47	0.48
1:B:493:ARG:HG2	1:B:510:LEU:HD11	1.96	0.48
1:A:149:ARG:HB3	1:A:158:PRO:CA	2.43	0.48
1:C:379:MSE:HE3	1:C:391:PRO:CB	2.43	0.48
1:A:340:PRO:O	1:A:342:ALA:N	2.46	0.48
1:D:235:LEU:CD2	1:D:235:LEU:H	2.25	0.48
1:D:436:LEU:HD21	1:D:478:LEU:HD22	1.96	0.48
1:A:197:ARG:HH11	1:A:197:ARG:HG2	1.78	0.48
1:D:245:PHE:CE1	1:D:252:VAL:HG22	2.48	0.48
1:C:340:PRO:O	1:C:341:ALA:C	2.52	0.48
1:C:352:ARG:CZ	1:C:373:GLY:HA3	2.44	0.48
1:D:18:GLN:NE2	1:D:37:THR:HA	2.19	0.48
1:C:26:ALA:HB1	1:C:125:LEU:CD2	2.44	0.48
1:B:349:LEU:HD12	1:B:349:LEU:N	2.29	0.48
1:A:312:ARG:HG2	1:A:313:ASP:N	2.28	0.48
1:B:45:GLU:OE2	1:B:98:THR:HG23	2.14	0.48
1:B:12:ARG:HB2	1:B:12:ARG:NH1	2.28	0.48
1:A:120:VAL:HG22	1:A:131:ALA:HB3	1.96	0.48
1:C:101:ASP:HB3	1:C:104:TRP:HB3	1.95	0.48
1:A:54:ILE:C	1:A:54:ILE:HD12	2.34	0.48
1:D:466:GLU:OE1	1:D:466:GLU:HA	2.14	0.48
1:B:193:LEU:HD13	1:B:208:ASP:CG	2.34	0.48
1:C:490:ASN:O	1:C:494:GLU:HG2	2.14	0.48
1:C:312:ARG:HD3	1:C:314:TRP:CE2	2.48	0.48
1:D:150:TRP:NE1	1:D:159:VAL:HG11	2.28	0.48
1:D:302:ARG:O	1:D:305:MSE:HB2	2.14	0.48
1:A:113:ILE:CG2	1:A:115:VAL:HG13	2.39	0.48
1:D:109:ILE:HG22	1:D:113:ILE:CG2	2.44	0.48
1:D:442:ARG:HH12	1:D:527:GLU:CD	2.16	0.48
1:D:366:LEU:HB3	1:D:368:LEU:HD13	1.96	0.48
1:D:536:LEU:HA	1:D:539:MSE:HE3	1.95	0.48
1:D:503:PRO:O	1:D:504:PHE:HB3	2.14	0.48
1:C:245:PHE:HB2	1:C:325:ILE:HD13	1.95	0.48
1:D:490:ASN:HD22	1:D:490:ASN:N	2.12	0.48
1:C:168:GLN:HG3	1:C:169:ARG:N	2.29	0.48
1:B:412:LEU:H	1:B:412:LEU:HD22	1.79	0.48
1:B:316:ARG:HB3	1:B:316:ARG:HH11	1.78	0.48
1:C:411:VAL:HG23	1:C:411:VAL:O	2.14	0.47
1:B:95:ILE:HG21	1:B:127:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:CG2	1:A:125:LEU:H	2.27	0.47
1:A:422:VAL:HA	1:A:423:PRO:C	2.33	0.47
1:A:165:TRP:CZ3	1:A:168:GLN:HG2	2.49	0.47
1:C:230:LEU:O	1:C:264:CYS:HB2	2.13	0.47
1:D:270:TYR:O	1:D:273:GLN:HB2	2.14	0.47
1:A:246:ASP:CB	1:A:253:LEU:HD11	2.44	0.47
1:A:87:GLY:C	1:A:88:ILE:HD12	2.34	0.47
1:B:422:VAL:O	1:B:472:THR:HG22	2.14	0.47
1:D:75:MSE:HG2	1:D:134:VAL:CG1	2.45	0.47
1:A:413:PRO:O	1:A:416:GLU:HG3	2.13	0.47
1:C:313:ASP:C	1:C:315:ASN:H	2.18	0.47
1:B:113:ILE:HG23	1:B:115:VAL:CG1	2.44	0.47
1:B:23:LEU:HD22	1:B:124:VAL:HG13	1.94	0.47
1:A:106:ARG:HG3	1:A:119:VAL:HG12	1.96	0.47
1:D:241:GLU:O	1:D:322:VAL:HG12	2.14	0.47
1:C:59:PRO:O	1:C:100:LEU:HA	2.15	0.47
1:B:443:PRO:HA	1:B:509:TYR:CZ	2.49	0.47
1:A:180:VAL:HG22	4:A:602:HOH:O	2.15	0.47
1:B:43:LYS:O	1:B:86:VAL:HA	2.15	0.47
1:D:124:VAL:C	1:D:126:GLY:H	2.17	0.47
1:D:341:ALA:O	1:D:342:ALA:CB	2.63	0.47
1:A:16:ILE:O	1:A:20:GLU:HG2	2.15	0.47
1:B:551:VAL:HG11	1:B:571:TYR:CE2	2.50	0.47
1:B:382:ALA:O	1:B:386:LEU:HD13	2.15	0.47
1:D:518:THR:HG23	1:D:554:LEU:HD11	1.96	0.47
1:D:150:TRP:O	1:D:156:CYS:HB2	2.15	0.47
1:B:211:LEU:HD23	1:B:211:LEU:C	2.35	0.47
1:B:503:PRO:O	1:B:504:PHE:HB2	2.15	0.47
1:A:314:TRP:HA	1:A:314:TRP:CE3	2.50	0.47
1:C:366:LEU:C	1:C:368:LEU:HD13	2.35	0.47
1:B:517:LEU:HD21	1:B:542:VAL:HG21	1.96	0.47
1:B:338:GLY:HA2	1:B:401:VAL:CG2	2.45	0.47
1:D:490:ASN:O	1:D:494:GLU:HG2	2.15	0.47
1:A:357:PRO:HD2	3:A:584:CL:CL	2.52	0.47
1:B:316:ARG:HH12	1:B:318:GLU:CD	2.17	0.47
1:A:274:ALA:O	1:A:278:VAL:HG23	2.15	0.47
1:B:567:ARG:HH11	1:B:567:ARG:HG2	1.79	0.47
1:B:148:LEU:O	1:B:148:LEU:HD12	2.15	0.47
1:C:381:GLN:CG	1:C:382:ALA:N	2.78	0.47
1:D:534:SER:HA	1:D:537:MSE:CE	2.43	0.47
1:C:152:VAL:HG21	1:C:157:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ILE:HD13	1:A:481:ALA:H	1.80	0.47
1:D:151:ARG:HH11	1:D:151:ARG:CG	2.28	0.46
1:A:333:VAL:O	1:A:402:GLU:HA	2.15	0.46
1:A:218:LEU:HD11	1:A:222:GLY:HA2	1.97	0.46
1:D:240:ILE:HG21	1:D:309:MSE:HE1	1.95	0.46
1:C:151:ARG:HH11	1:C:151:ARG:CG	2.28	0.46
1:B:15:LEU:O	1:B:19:VAL:HG23	2.15	0.46
1:B:197:ARG:NH1	1:B:197:ARG:HG2	2.29	0.46
1:A:271:LEU:HB3	1:A:305:MSE:CE	2.44	0.46
1:D:312:ARG:HG2	1:D:313:ASP:N	2.31	0.46
1:B:352:ARG:HD2	1:B:372:GLN:HG3	1.97	0.46
1:B:340:PRO:HG2	1:B:343:ILE:HG12	1.96	0.46
1:C:437:TYR:HA	1:C:440:PHE:CD2	2.50	0.46
1:A:421:ILE:HB	1:A:427:GLN:HG2	1.97	0.46
1:D:530:ASP:HB3	1:D:570:ARG:HB3	1.97	0.46
1:B:33:LYS:HD2	1:B:42:PHE:CE1	2.51	0.46
1:C:12:ARG:NH1	1:C:12:ARG:HB2	2.31	0.46
1:C:308:ALA:O	1:C:312:ARG:HB2	2.15	0.46
1:C:240:ILE:CG1	1:C:320:ILE:HB	2.42	0.46
1:B:48:ARG:NH2	1:B:97:GLY:O	2.48	0.46
1:A:27:ALA:O	1:A:28:ASP:HB2	2.16	0.46
1:D:250:GLY:O	1:D:251:GLN:CB	2.63	0.46
1:B:347:ASN:C	1:B:347:ASN:HD22	2.18	0.46
1:D:26:ALA:HB1	1:D:125:LEU:CD2	2.43	0.46
1:B:452:ARG:HB2	1:B:452:ARG:CZ	2.45	0.46
1:B:280:LYS:HD3	1:B:326:GLU:OE1	2.16	0.46
1:D:104:TRP:HA	1:D:459:GLU:HG2	1.97	0.46
1:B:75:MSE:HE2	1:B:82:GLY:HA3	1.98	0.46
1:D:537:MSE:O	1:D:541:GLY:HA2	2.16	0.46
1:B:275:LEU:HD23	1:B:301:VAL:CG1	2.45	0.46
1:A:55:GLU:HB3	1:A:56:PRO:HD2	1.98	0.46
1:B:43:LYS:HE3	1:B:71:GLU:OE1	2.15	0.46
1:C:431:ARG:HH11	1:C:463:ASN:HD21	1.64	0.46
1:C:231:LEU:HD22	1:C:362:LEU:HD23	1.98	0.46
1:A:58:LYS:HB3	1:A:59:PRO:HD2	1.97	0.46
1:C:312:ARG:NH1	1:C:314:TRP:N	2.61	0.46
1:D:280:LYS:O	1:D:281:ASN:CB	2.58	0.46
1:C:113:ILE:HG23	1:C:115:VAL:H	1.79	0.46
1:D:98:THR:HG21	1:D:100:LEU:HD12	1.97	0.46
1:D:124:VAL:HG23	1:D:125:LEU:H	1.81	0.46
1:C:491:ALA:O	1:C:495:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:PRO:HG2	1:D:499:VAL:HG22	1.95	0.45
1:D:312:ARG:HG2	1:D:312:ARG:HH11	1.81	0.45
1:B:149:ARG:HB2	1:B:157:ARG:O	2.15	0.45
1:B:438:LEU:HD13	1:B:445:ILE:HD11	1.98	0.45
1:C:396:ILE:CG2	1:C:397:ALA:N	2.79	0.45
1:A:106:ARG:HG3	1:A:119:VAL:CG1	2.46	0.45
1:B:161:ARG:NH2	1:B:361:ASP:OD1	2.49	0.45
1:D:473:VAL:HG21	1:D:492:CYS:SG	2.56	0.45
1:C:281:ASN:HB2	1:C:294:PRO:HA	1.98	0.45
1:D:432:ILE:CD1	1:D:436:LEU:HD12	2.46	0.45
1:B:521:ALA:HB1	1:B:531:LEU:CD2	2.47	0.45
1:B:259:GLU:HB3	1:B:261:GLU:OE2	2.16	0.45
1:B:466:GLU:O	1:B:470:GLN:HG3	2.15	0.45
1:D:257:VAL:O	1:D:257:VAL:HG23	2.15	0.45
1:D:280:LYS:HE3	4:D:651:HOH:O	2.15	0.45
1:C:114:ASP:CG	1:C:371:LYS:HE3	2.36	0.45
1:C:422:VAL:HG13	1:C:423:PRO:HA	1.97	0.45
1:B:148:LEU:C	1:B:148:LEU:HD12	2.37	0.45
1:B:139:GLU:HB2	1:B:140:PRO:HD2	1.99	0.45
1:C:149:ARG:HB2	1:C:157:ARG:O	2.16	0.45
1:D:259:GLU:HB3	1:D:261:GLU:OE2	2.17	0.45
1:A:348:VAL:HG23	1:A:349:LEU:HD12	1.99	0.45
1:B:559:ARG:HD2	4:B:586:HOH:O	2.15	0.45
1:D:344:THR:HG23	1:D:346:GLU:H	1.81	0.45
1:C:447:ILE:HG22	4:C:652:HOH:O	2.16	0.45
1:B:109:ILE:HG22	1:B:113:ILE:CG2	2.46	0.45
1:B:322:VAL:HA	1:B:332:ILE:O	2.16	0.45
1:B:418:VAL:O	1:B:421:ILE:HG12	2.16	0.45
1:A:166:GLU:OE1	1:B:166:GLU:OE1	2.34	0.45
1:C:371:LYS:O	1:C:372:GLN:HB2	2.17	0.45
1:D:235:LEU:HD23	1:D:235:LEU:N	2.30	0.45
1:A:380:TYR:CE2	1:A:391:PRO:HG2	2.52	0.45
1:A:178:ALA:HB2	1:A:358:ALA:HB2	1.98	0.45
1:A:439:LEU:HD13	1:A:488:LEU:N	2.32	0.45
1:A:172:SER:HA	4:A:615:HOH:O	2.16	0.45
1:D:218:LEU:HD11	1:D:222:GLY:HA2	1.98	0.45
1:A:439:LEU:HD21	1:A:445:ILE:HB	1.98	0.45
1:C:189:ARG:NH2	1:C:262:LYS:HA	2.32	0.45
1:D:519:ASN:HD22	1:D:519:ASN:HA	1.56	0.45
1:D:241:GLU:CB	1:D:257:VAL:HG12	2.42	0.44
1:D:46:ALA:HB3	1:D:64:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ILE:HG22	1:D:397:ALA:H	1.80	0.44
1:C:197:ARG:HG2	1:C:197:ARG:NH1	2.32	0.44
1:B:18:GLN:O	1:B:22:ILE:HG13	2.16	0.44
1:B:318:GLU:HA	1:B:319:PRO:HD3	1.78	0.44
1:D:551:VAL:HG11	1:D:571:TYR:CE2	2.52	0.44
1:B:312:ARG:HG2	1:B:313:ASP:N	2.32	0.44
1:B:26:ALA:HB1	1:B:125:LEU:HD21	1.97	0.44
1:D:151:ARG:CB	1:D:151:ARG:HH11	2.27	0.44
1:B:88:ILE:HD11	1:B:129:VAL:HG11	1.98	0.44
1:B:235:LEU:HD23	1:B:235:LEU:N	2.26	0.44
1:B:233:THR:HG23	4:B:591:HOH:O	2.18	0.44
1:C:429:ASP:O	1:C:432:ILE:HG13	2.18	0.44
1:B:89:GLU:OE2	1:B:94:ARG:HD2	2.17	0.44
1:C:376:VAL:O	1:C:379:MSE:HB3	2.17	0.44
1:D:106:ARG:HG3	1:D:119:VAL:CG1	2.47	0.44
1:B:275:LEU:HD23	1:B:301:VAL:HG11	2.00	0.44
1:D:150:TRP:NE1	1:D:159:VAL:CG1	2.81	0.44
1:B:313:ASP:O	1:B:315:ASN:N	2.51	0.44
1:B:37:THR:O	1:B:40:VAL:HG23	2.17	0.44
1:D:85:ILE:HG21	1:D:88:ILE:HD12	1.98	0.44
1:D:490:ASN:HA	1:D:493:ARG:HD2	1.99	0.44
1:B:250:GLY:O	1:B:251:GLN:CB	2.64	0.44
1:D:256:VAL:HG13	1:D:256:VAL:O	2.18	0.44
1:D:95:ILE:HG21	1:D:127:GLN:HB2	2.00	0.44
1:A:242:LEU:HB2	1:A:271:LEU:HD11	1.98	0.44
1:A:366:LEU:HB3	1:A:368:LEU:HD13	1.99	0.44
1:B:48:ARG:NH1	1:B:57:GLY:N	2.66	0.44
1:B:225:SER:O	1:B:226:GLN:C	2.56	0.44
1:C:109:ILE:HG22	1:C:113:ILE:HG21	1.98	0.44
1:A:312:ARG:HD3	1:A:314:TRP:CE2	2.51	0.44
1:C:163:GLU:O	1:C:166:GLU:HG2	2.18	0.44
1:C:113:ILE:O	1:C:114:ASP:HB2	2.18	0.44
1:D:522:MSE:CE	1:D:573:LEU:HD23	2.48	0.44
1:A:237:ARG:HG2	1:A:237:ARG:HH21	1.83	0.44
1:B:532:ALA:HB2	1:B:570:ARG:NE	2.26	0.43
1:B:19:VAL:HG13	1:B:85:ILE:CD1	2.46	0.43
1:C:440:PHE:CE1	1:C:496:LEU:HD21	2.52	0.43
1:A:124:VAL:CG2	1:A:125:LEU:N	2.79	0.43
1:B:525:LEU:CD2	1:B:531:LEU:HB3	2.48	0.43
1:B:69:ALA:O	1:B:113:ILE:HD12	2.18	0.43
1:B:323:ARG:HG3	1:B:332:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:NH1	1:A:55:GLU:O	2.51	0.43
1:B:428:ASP:HA	4:B:622:HOH:O	2.17	0.43
1:C:124:VAL:HG23	1:C:125:LEU:N	2.33	0.43
1:C:73:ALA:CA	1:C:113:ILE:HD11	2.47	0.43
1:B:124:VAL:HG23	1:B:125:LEU:H	1.83	0.43
1:B:30:ARG:CB	1:B:94:ARG:HA	2.48	0.43
1:B:235:LEU:HD11	1:B:239:ALA:HB2	2.00	0.43
1:A:432:ILE:HD12	1:A:433:ALA:N	2.32	0.43
1:A:310:ILE:HD11	1:A:369:VAL:HG21	2.00	0.43
1:C:179:GLN:HG2	1:C:180:VAL:N	2.34	0.43
1:A:219:ASP:HB2	1:A:223:PHE:O	2.18	0.43
1:C:313:ASP:O	1:C:315:ASN:N	2.49	0.43
1:B:337:GLY:O	1:B:401:VAL:HG23	2.19	0.43
1:A:465:LEU:HD13	1:A:486:TRP:CZ3	2.53	0.43
1:C:279:ASN:HD21	1:C:296:ILE:H	1.67	0.43
1:D:151:ARG:HA	1:D:156:CYS:CB	2.44	0.43
1:B:312:ARG:NH1	1:B:314:TRP:N	2.67	0.43
1:A:411:VAL:O	1:A:411:VAL:HG13	2.19	0.43
1:C:11:ARG:HG3	1:C:11:ARG:NH2	2.33	0.43
1:B:268:LEU:O	1:B:272:GLU:HG3	2.19	0.43
1:D:379:MSE:O	1:D:382:ALA:HB3	2.19	0.43
1:A:75:MSE:O	1:A:78:THR:HG23	2.19	0.43
1:B:12:ARG:HB2	1:B:12:ARG:HH11	1.84	0.43
1:A:83:ALA:C	1:A:84:LEU:HD12	2.39	0.43
1:D:442:ARG:NH1	1:D:527:GLU:OE2	2.49	0.43
1:D:323:ARG:O	1:D:331:LEU:HD12	2.19	0.43
1:C:177:MSE:HE2	1:C:356:TYR:CD1	2.52	0.43
1:B:313:ASP:OD2	1:B:315:ASN:HB2	2.19	0.43
1:C:366:LEU:HB3	1:C:368:LEU:CD1	2.47	0.43
1:C:247:VAL:HA	1:C:325:ILE:HG23	2.01	0.43
1:D:318:GLU:HA	1:D:319:PRO:HD3	1.81	0.43
1:A:287:GLY:C	1:A:289:VAL:H	2.22	0.43
1:A:312:ARG:NH2	1:A:318:GLU:O	2.52	0.43
1:D:525:LEU:HD21	1:D:531:LEU:HB3	2.01	0.43
1:D:445:ILE:HD11	1:D:449:VAL:CG1	2.48	0.43
1:A:74:CYS:O	1:A:78:THR:CG2	2.67	0.43
1:D:157:ARG:HB3	1:D:158:PRO:HD2	1.99	0.43
1:B:380:TYR:O	1:B:384:ILE:HG12	2.19	0.43
1:B:231:LEU:HD11	1:B:363:TYR:OH	2.19	0.43
1:D:75:MSE:SE	1:D:82:GLY:HA3	2.69	0.43
1:A:346:GLU:HB3	4:A:662:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:ARG:O	1:D:497:ARG:HG3	2.19	0.43
1:C:48:ARG:NH1	1:C:57:GLY:N	2.67	0.43
1:D:124:VAL:HG23	1:D:125:LEU:N	2.34	0.42
1:B:426:ARG:NH2	1:B:426:ARG:HG2	2.33	0.42
1:A:34:THR:O	1:A:35:LYS:C	2.57	0.42
1:D:278:VAL:C	1:D:280:LYS:H	2.21	0.42
1:A:271:LEU:O	1:A:275:LEU:HB2	2.19	0.42
1:C:84:LEU:HD12	1:C:84:LEU:N	2.34	0.42
1:C:60:GLU:HG2	1:C:104:TRP:CG	2.54	0.42
1:C:242:LEU:HA	1:C:322:VAL:O	2.19	0.42
1:A:434:ILE:HG13	1:A:454:LEU:HD23	2.00	0.42
1:B:429:ASP:C	1:B:429:ASP:OD2	2.57	0.42
1:B:470:GLN:HE22	1:D:57:GLY:N	1.93	0.42
1:B:455:GLN:HB3	1:B:455:GLN:HE21	1.63	0.42
1:C:44:GLU:O	1:C:45:GLU:C	2.56	0.42
1:B:517:LEU:HD22	1:B:536:LEU:HD11	2.00	0.42
1:D:58:LYS:HB3	1:D:59:PRO:HD2	2.01	0.42
1:D:422:VAL:HA	1:D:423:PRO:C	2.40	0.42
1:B:165:TRP:CE3	1:B:168:GLN:HG2	2.54	0.42
1:D:525:LEU:HB3	1:D:573:LEU:HG	2.01	0.42
1:D:522:MSE:HA	1:D:525:LEU:HD12	2.02	0.42
1:C:165:TRP:CE3	1:C:168:GLN:HG2	2.54	0.42
1:B:364:ARG:HG2	1:B:369:VAL:HG23	2.00	0.42
1:B:439:LEU:CD1	1:B:479:ILE:HG22	2.49	0.42
1:D:242:LEU:HB2	1:D:271:LEU:HD11	2.01	0.42
1:B:242:LEU:HA	1:B:322:VAL:O	2.20	0.42
1:A:95:ILE:HG21	1:A:127:GLN:HB2	2.01	0.42
1:D:73:ALA:HB2	1:D:113:ILE:HD11	2.00	0.42
1:B:168:GLN:O	1:B:172:SER:HB2	2.19	0.42
1:D:250:GLY:O	1:D:251:GLN:HB3	2.19	0.42
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.84	0.42
1:D:352:ARG:CZ	1:D:373:GLY:HA3	2.49	0.42
1:D:281:ASN:HB2	1:D:294:PRO:HA	2.00	0.42
1:B:242:LEU:HB2	1:B:271:LEU:CD1	2.48	0.42
1:B:78:THR:CG2	1:B:151:ARG:H	2.32	0.42
1:B:148:LEU:CD1	1:B:159:VAL:HG23	2.49	0.42
1:A:328:ASP:CB	1:A:330:THR:HG23	2.49	0.42
1:C:168:GLN:O	1:C:172:SER:HB2	2.20	0.42
1:A:369:VAL:HG12	1:A:370:ASP:N	2.34	0.42
1:B:383:MSE:HG3	1:B:391:PRO:HD3	2.01	0.42
1:D:177:MSE:HA	1:D:226:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LYS:HB3	4:D:597:HOH:O	2.20	0.42
1:C:230:LEU:HD12	1:C:230:LEU:O	2.20	0.42
1:B:381:GLN:HG3	1:B:382:ALA:N	2.34	0.42
1:D:218:LEU:HD13	1:D:219:ASP:O	2.20	0.42
1:B:560:VAL:HG12	1:B:573:LEU:HA	2.02	0.42
1:A:362:LEU:O	1:A:366:LEU:CD2	2.68	0.42
1:C:205:GLU:OE1	1:D:91:LYS:HE3	2.20	0.42
1:A:247:VAL:O	1:A:249:GLY:N	2.53	0.42
1:B:189:ARG:HD3	1:B:266:GLU:OE1	2.20	0.42
1:D:417:LEU:HD21	1:D:492:CYS:SG	2.60	0.42
1:B:85:ILE:CG2	1:B:88:ILE:HD13	2.45	0.42
1:B:313:ASP:C	1:B:315:ASN:H	2.23	0.42
1:B:95:ILE:O	1:D:423:PRO:HB3	2.20	0.42
1:A:26:ALA:HB1	1:A:125:LEU:HD12	2.01	0.42
1:A:98:THR:HG23	1:A:130:LEU:HD22	2.01	0.42
1:D:376:VAL:O	1:D:379:MSE:HB3	2.19	0.42
1:D:114:ASP:CG	1:D:352:ARG:HD2	2.41	0.42
1:C:19:VAL:HG13	1:C:85:ILE:HD11	2.01	0.42
1:B:513:ASP:OD2	1:B:515:ALA:HB3	2.19	0.42
1:B:374:VAL:HG12	1:B:378:ARG:HD3	2.02	0.42
1:C:178:ALA:HB2	1:C:358:ALA:CB	2.49	0.42
1:B:113:ILE:O	1:B:114:ASP:HB2	2.20	0.42
1:A:69:ALA:O	1:A:113:ILE:HD12	2.20	0.42
1:B:241:GLU:O	1:B:322:VAL:HG12	2.20	0.42
1:B:88:ILE:N	1:B:88:ILE:HD12	2.35	0.42
1:A:125:LEU:HD12	1:A:125:LEU:N	2.35	0.42
1:A:423:PRO:HG2	1:A:426:ARG:HG3	2.01	0.42
1:A:140:PRO:HG2	1:A:361:ASP:OD1	2.20	0.42
1:B:165:TRP:HB3	1:B:169:ARG:NH1	2.34	0.42
1:C:334:ARG:HG3	1:C:334:ARG:NH1	2.35	0.42
1:B:270:TYR:O	1:B:273:GLN:HB2	2.20	0.42
1:A:193:LEU:HD13	1:A:208:ASP:CG	2.40	0.42
1:D:421:ILE:HD13	1:D:473:VAL:CG1	2.49	0.41
1:B:75:MSE:HB3	1:B:134:VAL:HG11	2.01	0.41
1:A:318:GLU:HA	1:A:319:PRO:HD3	1.79	0.41
1:C:235:LEU:H	1:C:235:LEU:HD23	1.85	0.41
1:B:560:VAL:HG12	1:B:573:LEU:CA	2.50	0.41
1:C:278:VAL:HG12	1:C:324:TRP:CD1	2.55	0.41
1:A:386:LEU:HD13	4:A:621:HOH:O	2.20	0.41
1:D:380:TYR:O	1:D:381:GLN:C	2.59	0.41
1:C:275:LEU:HD23	1:C:305:MSE:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:LEU:HD22	1:D:536:LEU:HD11	2.02	0.41
1:B:316:ARG:HH11	1:B:316:ARG:CB	2.33	0.41
1:B:195:LEU:HB3	1:B:199:TRP:CH2	2.55	0.41
1:C:45:GLU:OE2	1:C:98:THR:HG23	2.20	0.41
1:D:344:THR:CG2	1:D:347:ASN:HD22	2.33	0.41
1:B:551:VAL:O	1:B:555:VAL:HG23	2.20	0.41
1:C:337:GLY:O	1:C:401:VAL:HG23	2.21	0.41
1:C:75:MSE:HE3	1:C:78:THR:OG1	2.20	0.41
1:A:73:ALA:O	1:A:77:ASN:ND2	2.54	0.41
1:B:421:ILE:HB	1:B:427:GLN:HG3	2.01	0.41
1:B:230:LEU:HD23	1:B:231:LEU:HD13	2.02	0.41
1:D:306:LEU:HA	1:D:309:MSE:CB	2.50	0.41
1:B:496:LEU:HB3	1:B:507:VAL:CG2	2.51	0.41
1:C:61:ASN:ND2	1:C:64:ALA:H	2.19	0.41
1:A:275:LEU:HA	1:A:275:LEU:HD12	1.82	0.41
1:D:177:MSE:HE2	1:D:356:TYR:CG	2.55	0.41
1:C:268:LEU:HD13	1:C:309:MSE:HE3	2.02	0.41
1:D:443:PRO:HA	1:D:509:TYR:CE2	2.56	0.41
1:C:490:ASN:HD22	1:C:490:ASN:HA	1.66	0.41
1:B:447:ILE:HG23	1:B:448:ASP:N	2.35	0.41
1:B:177:MSE:HE2	1:B:356:TYR:CG	2.56	0.41
1:B:312:ARG:HG2	1:B:313:ASP:H	1.86	0.41
1:A:231:LEU:HD22	1:A:362:LEU:HD23	2.01	0.41
1:B:418:VAL:HA	1:B:421:ILE:HG12	2.03	0.41
1:A:370:ASP:O	1:A:371:LYS:C	2.58	0.41
1:B:279:ASN:ND2	1:B:324:TRP:HH2	2.18	0.41
1:A:452:ARG:HB2	1:A:452:ARG:HH21	1.84	0.41
1:B:472:THR:CG2	1:D:127:GLN:HE21	2.25	0.41
1:A:73:ALA:CA	1:A:113:ILE:HD11	2.51	0.41
1:A:115:VAL:HG22	1:A:117:PRO:HD3	2.03	0.41
1:B:381:GLN:HB2	1:B:381:GLN:HE21	1.69	0.41
1:A:371:LYS:O	1:A:372:GLN:HB2	2.20	0.41
1:D:110:PHE:HB2	1:D:116:ALA:HB2	2.03	0.41
1:D:281:ASN:C	1:D:281:ASN:ND2	2.73	0.41
1:D:163:GLU:HA	1:D:166:GLU:OE1	2.21	0.41
1:B:298:ARG:HH21	1:B:298:ARG:CG	2.33	0.41
1:C:123:ARG:HA	1:C:127:GLN:O	2.21	0.41
1:D:237:ARG:HB3	4:D:635:HOH:O	2.20	0.41
1:D:420:SER:HB3	4:D:598:HOH:O	2.21	0.41
1:C:432:ILE:HD11	4:C:598:HOH:O	2.21	0.41
1:D:306:LEU:HA	1:D:309:MSE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:H	1:A:412:LEU:CD2	2.32	0.41
1:C:443:PRO:HG2	1:C:444:PHE:H	1.85	0.41
1:B:352:ARG:HA	1:B:372:GLN:HG2	2.03	0.41
1:A:50:ASN:O	1:A:50:ASN:OD1	2.39	0.41
1:B:330:THR:HG22	1:B:406:VAL:HG13	2.02	0.41
1:B:431:ARG:HH12	1:B:463:ASN:HD21	1.68	0.41
1:A:241:GLU:HB2	1:A:257:VAL:HG12	2.03	0.41
1:B:349:LEU:HD13	1:B:455:GLN:OE1	2.21	0.41
1:A:313:ASP:OD1	1:A:316:ARG:HD2	2.20	0.41
1:C:219:ASP:HB2	1:C:223:PHE:O	2.21	0.41
1:A:68:LEU:O	1:A:72:VAL:HG23	2.21	0.41
1:C:119:VAL:HA	1:C:131:ALA:O	2.21	0.41
1:C:432:ILE:HD12	1:C:433:ALA:CA	2.51	0.40
1:B:411:VAL:HG22	1:B:413:PRO:HG2	2.03	0.40
1:B:432:ILE:HD12	1:B:433:ALA:N	2.36	0.40
1:D:363:TYR:HB3	1:D:369:VAL:HG23	2.03	0.40
1:C:439:LEU:HD13	1:C:488:LEU:HD13	2.03	0.40
1:A:78:THR:HG21	1:A:151:ARG:H	1.84	0.40
1:A:234:SER:CB	1:A:261:GLU:O	2.58	0.40
1:D:108:GLY:O	1:D:112:ARG:CD	2.59	0.40
1:D:242:LEU:HA	1:D:322:VAL:HG13	2.03	0.40
1:A:157:ARG:HB3	1:A:158:PRO:HD2	2.02	0.40
1:A:152:VAL:CG2	1:A:157:ARG:HD3	2.48	0.40
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.81	0.40
1:C:165:TRP:O	1:C:169:ARG:HG3	2.21	0.40
1:A:291:LYS:HB2	1:A:291:LYS:HE3	1.91	0.40
1:A:296:ILE:CG2	1:A:407:GLY:HA3	2.37	0.40
1:B:148:LEU:HD12	1:B:159:VAL:HG23	2.03	0.40
1:C:443:PRO:HG2	1:C:444:PHE:N	2.37	0.40
1:A:180:VAL:HG23	4:A:638:HOH:O	2.21	0.40
1:B:174:PHE:CZ	1:B:176:PRO:HA	2.57	0.40
1:A:135:ALA:HA	4:A:643:HOH:O	2.20	0.40
1:B:534:SER:HA	1:B:537:MSE:CE	2.38	0.40
1:B:127:GLN:NE2	1:D:472:THR:HG22	2.37	0.40
1:C:473:VAL:HG11	1:C:492:CYS:SG	2.61	0.40
1:C:436:LEU:HA	1:C:436:LEU:HD23	1.83	0.40
1:D:337:GLY:O	1:D:401:VAL:HG23	2.22	0.40
1:A:280:LYS:HE3	1:A:326:GLU:OE1	2.22	0.40
1:B:471:THR:HB	1:B:478:LEU:HD12	2.02	0.40
1:D:70:ASP:OD2	1:D:143:ASP:HB2	2.22	0.40
1:A:119:VAL:HA	1:A:131:ALA:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:GLN:HB2	1:A:442:ARG:H	1.71	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	490/583 (84%)	432 (88%)	46 (9%)	12 (2%)	7	35
1	B	551/583 (94%)	488 (89%)	51 (9%)	12 (2%)	8	38
1	C	473/583 (81%)	431 (91%)	30 (6%)	12 (2%)	7	34
1	D	552/583 (95%)	492 (89%)	51 (9%)	9 (2%)	12	48
All	All	2066/2332 (89%)	1843 (89%)	178 (9%)	45 (2%)	8	38

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	ALA
1	A	342	ALA
1	B	280	LYS
1	B	341	ALA
1	B	342	ALA
1	B	372	GLN
1	C	280	LYS
1	C	341	ALA
1	C	342	ALA
1	D	280	LYS
1	D	341	ALA
1	D	342	ALA
1	A	124	VAL
1	A	219	ASP

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Mol	Chain	Res	Type
1	A	248	HIS
1	A	280	LYS
1	A	372	GLN
1	B	102	ILE
1	B	113	ILE
1	B	124	VAL
1	B	248	HIS
1	B	251	GLN
1	C	124	VAL
1	C	312	ARG
1	C	372	GLN
1	D	124	VAL
1	D	251	GLN
1	D	372	GLN
1	A	314	TRP
1	B	314	TRP
1	C	204	ALA
1	C	248	HIS
1	C	314	TRP
1	A	249	GLY
1	A	251	GLN
1	C	249	GLY
1	A	236	ASP
1	C	251	GLN
1	A	398	GLY
1	D	305	MSE
1	B	250	GLY
1	B	152	VAL
1	D	152	VAL
1	D	153	GLY
1	C	340	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/462 (86%)	363 (92%)	33 (8%)	14	46
1	B	445/462 (96%)	405 (91%)	40 (9%)	12	41
1	C	382/462 (83%)	352 (92%)	30 (8%)	15	48
1	D	446/462 (96%)	406 (91%)	40 (9%)	12	41
All	All	1669/1848 (90%)	1526 (91%)	143 (9%)	13	44

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	15	LEU
1	A	48	ARG
1	A	49	ARG
1	A	61	ASN
1	A	68	LEU
1	A	78	THR
1	A	112	ARG
1	A	114	ASP
1	A	115	VAL
1	A	130	LEU
1	A	134	VAL
1	A	149	ARG
1	A	150	TRP
1	A	151	ARG
1	A	168	GLN
1	A	185	LEU
1	A	198	LYS
1	A	219	ASP
1	A	230	LEU
1	A	237	ARG
1	A	271	LEU
1	A	279	ASN
1	A	316	ARG
1	A	323	ARG
1	A	330	THR
1	A	359	LEU
1	A	381	GLN
1	A	404	THR
1	A	446	THR

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Mol	Chain	Res	Type
1	A	480	ILE
1	A	486	TRP
1	A	500	GLU
1	B	9	GLU
1	B	12	ARG
1	B	15	LEU
1	B	30	ARG
1	B	32	GLN
1	B	53	GLN
1	B	61	ASN
1	B	78	THR
1	B	112	ARG
1	B	114	ASP
1	B	149	ARG
1	B	150	TRP
1	B	151	ARG
1	B	159	VAL
1	B	167	TYR
1	B	168	GLN
1	B	206	LEU
1	B	218	LEU
1	B	230	LEU
1	B	231	LEU
1	B	271	LEU
1	B	279	ASN
1	B	281	ASN
1	B	307	ASN
1	B	316	ARG
1	B	328	ASP
1	B	334	ARG
1	B	347	ASN
1	B	364	ARG
1	B	366	LEU
1	B	370	ASP
1	B	381	GLN
1	B	404	THR
1	B	432	ILE
1	B	452	ARG
1	B	480	ILE
1	B	487	LEU
1	B	543	SER
1	B	567	ARG

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Mol	Chain	Res	Type
1	B	573	LEU
1	C	12	ARG
1	C	15	LEU
1	C	21	SER
1	C	28	ASP
1	C	61	ASN
1	C	68	LEU
1	C	78	THR
1	C	112	ARG
1	C	114	ASP
1	C	115	VAL
1	C	119	VAL
1	C	124	VAL
1	C	130	LEU
1	C	134	VAL
1	C	149	ARG
1	C	150	TRP
1	C	151	ARG
1	C	168	GLN
1	C	207	THR
1	C	218	LEU
1	C	271	LEU
1	C	279	ASN
1	C	323	ARG
1	C	330	THR
1	C	359	LEU
1	C	366	LEU
1	C	381	GLN
1	C	393	ILE
1	C	442	ARG
1	C	486	TRP
1	D	9	GLU
1	D	12	ARG
1	D	15	LEU
1	D	61	ASN
1	D	78	THR
1	D	112	ARG
1	D	115	VAL
1	D	134	VAL
1	D	146	ASP
1	D	149	ARG
1	D	150	TRP

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Mol	Chain	Res	Type
1	D	151	ARG
1	D	157	ARG
1	D	168	GLN
1	D	206	LEU
1	D	237	ARG
1	D	261	GLU
1	D	271	LEU
1	D	279	ASN
1	D	280	LYS
1	D	281	ASN
1	D	307	ASN
1	D	323	ARG
1	D	328	ASP
1	D	366	LEU
1	D	368	LEU
1	D	381	GLN
1	D	403	THR
1	D	432	ILE
1	D	446	THR
1	D	448	ASP
1	D	455	GLN
1	D	486	TRP
1	D	487	LEU
1	D	490	ASN
1	D	504	PHE
1	D	508	ARG
1	D	519	ASN
1	D	569	ARG
1	D	573	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	53	GLN
1	A	61	ASN
1	A	107	GLN
1	A	171	GLN
1	A	279	ASN
1	A	347	ASN
1	A	381	GLN
1	B	38	GLN

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Mol	Chain	Res	Type
1	B	61	ASN
1	B	107	GLN
1	B	179	GLN
1	B	279	ASN
1	B	281	ASN
1	B	347	ASN
1	B	381	GLN
1	B	388	HIS
1	B	455	GLN
1	B	463	ASN
1	B	470	GLN
1	B	490	ASN
1	B	519	ASN
1	C	53	GLN
1	C	61	ASN
1	C	279	ASN
1	C	347	ASN
1	C	381	GLN
1	C	463	ASN
1	C	490	ASN
1	D	14	GLN
1	D	18	GLN
1	D	38	GLN
1	D	50	ASN
1	D	53	GLN
1	D	61	ASN
1	D	107	GLN
1	D	127	GLN
1	D	279	ASN
1	D	281	ASN
1	D	347	ASN
1	D	381	GLN
1	D	441	GLN
1	D	463	ASN
1	D	490	ASN
1	D	519	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 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	486/583 (83%)	-0.40	0 <span>100</span> <span>100</span>	9, 29, 65, 98	0
1	B	546/583 (93%)	-0.40	2 (0%) <span>93</span> <span>80</span>	14, 45, 85, 119	0
1	C	471/583 (80%)	-0.40	0 <span>100</span> <span>100</span>	9, 34, 74, 103	0
1	D	547/583 (93%)	-0.35	1 (0%) <span>95</span> <span>87</span>	14, 47, 88, 126	0
All	All	2050/2332 (87%)	-0.39	3 (0%) <span>95</span> <span>90</span>	9, 39, 82, 126	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	567	ARG	3.0
1	B	341	ALA	2.5
1	B	567	ARG	2.5

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	CL	A	585	1/1	0.93	0.18	-0.60	71,71,71,71	0
3	CL	D	584	1/1	0.98	0.15	-0.73	47,47,47,47	0
2	CO	A	601	1/1	0.92	0.15	-1.11	93,93,93,93	0
3	CL	C	584	1/1	0.99	0.13	-2.15	37,37,37,37	0
2	CO	C	601	1/1	0.96	0.15	-2.40	106,106,106,106	0
2	CO	B	601	1/1	0.92	0.12	-2.58	88,88,88,88	0
3	CL	A	584	1/1	0.99	0.11	-3.50	28,28,28,28	0
2	CO	D	601	1/1	0.94	0.06	-3.88	93,93,93,93	0
3	CL	B	584	1/1	0.99	0.10	-4.39	40,40,40,40	0
3	CL	A	586	1/1	0.85	0.14	-	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.