



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2016 – 12:29 PM EST

PDB ID : 3WRW  
Title : Crystal structure of the N-terminal domain of resistance protein  
Authors : Katoh, E.; Kezuka, Y.  
Deposited on : 2014-02-27  
Resolution : 2.71 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
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) : rb-20028320

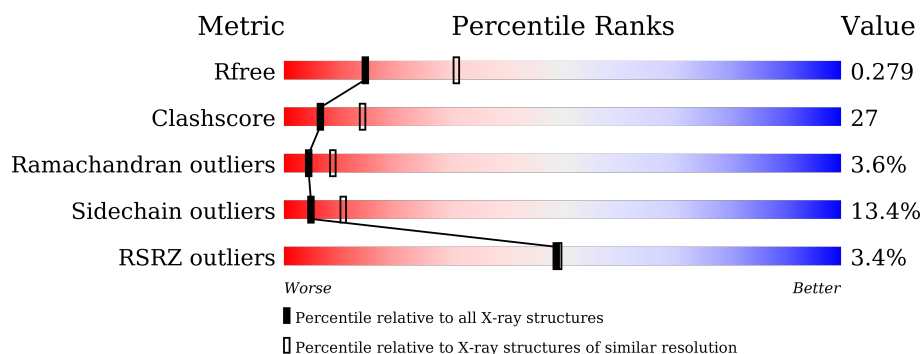
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	431	<div> <div>2%</div> <div>53% 35% 6% 6%</div> </div>
1	B	431	<div> <div>2%</div> <div>50% 37% 6% 6%</div> </div>
1	C	431	<div> <div>2%</div> <div>44% 39% 9% 7%</div> </div>
1	D	431	<div> <div>2%</div> <div>49% 35% 8% 7%</div> </div>
1	E	431	<div> <div>7%</div> <div>52% 31% 7% 10%</div> </div>
1	F	431	<div> <div>4%</div> <div>46% 34% 7% 12%</div> </div>

## 2 Entry composition [i](#)

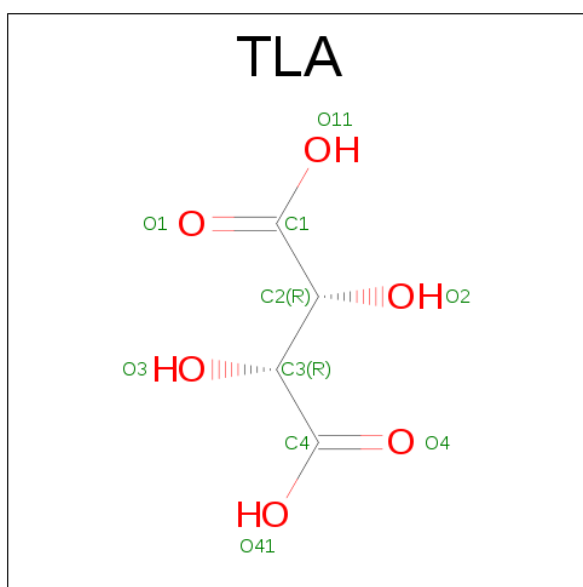
There are 3 unique types of molecules in this entry. The entry contains 17863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tm-1 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	Se	0	1	0
			3045	1927	507	592	10	9			
1	B	403	Total	C	N	O	S	Se	0	1	0
			3027	1914	504	591	10	8			
1	C	400	Total	C	N	O	S	Se	0	0	0
			2996	1895	498	585	10	8			
1	D	401	Total	C	N	O	S	Se	0	0	0
			3015	1910	503	584	10	8			
1	E	386	Total	C	N	O	S	Se	0	1	0
			2881	1829	473	561	10	8			
1	F	380	Total	C	N	O	S	Se	0	0	0
			2835	1794	466	557	10	8			

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

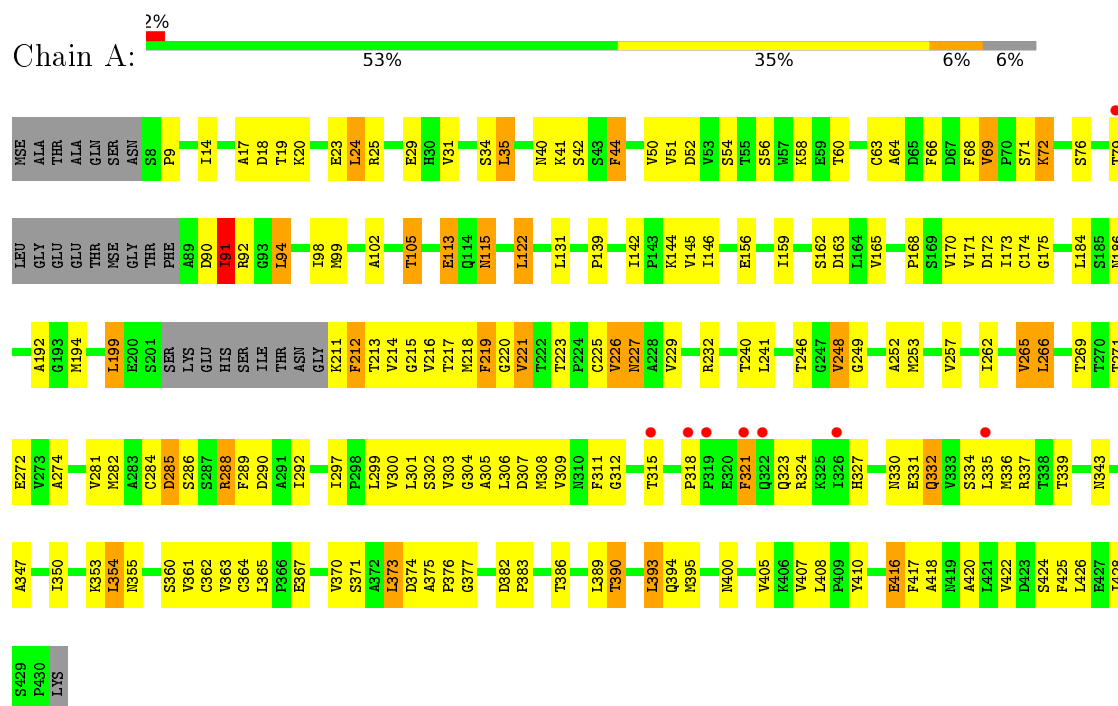
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	5	Total	O	0	0
			5	5		
3	C	12	Total	O	0	0
			12	12		
3	D	7	Total	O	0	0
			7	7		
3	E	8	Total	O	0	0
			8	8		
3	F	5	Total	O	0	0
			5	5		

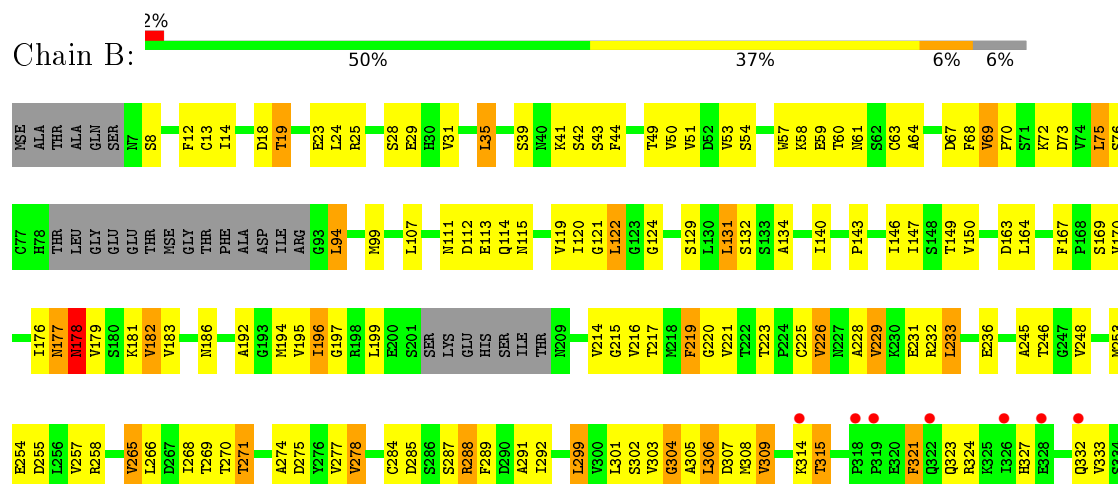
### 3 Residue-property plots

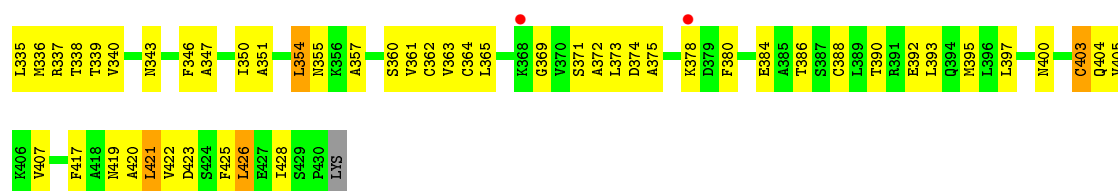
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Tm-1 protein

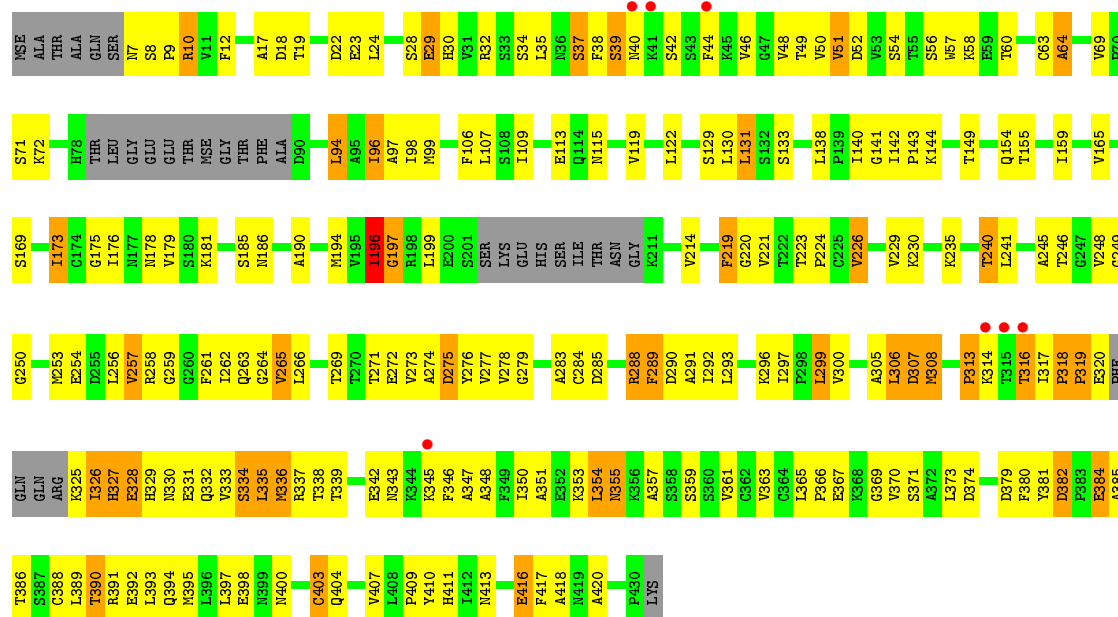
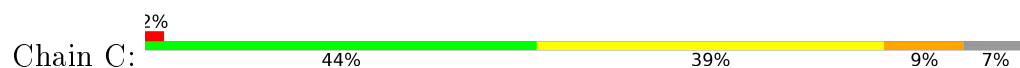


#### • Molecule 1: Tm-1 protein

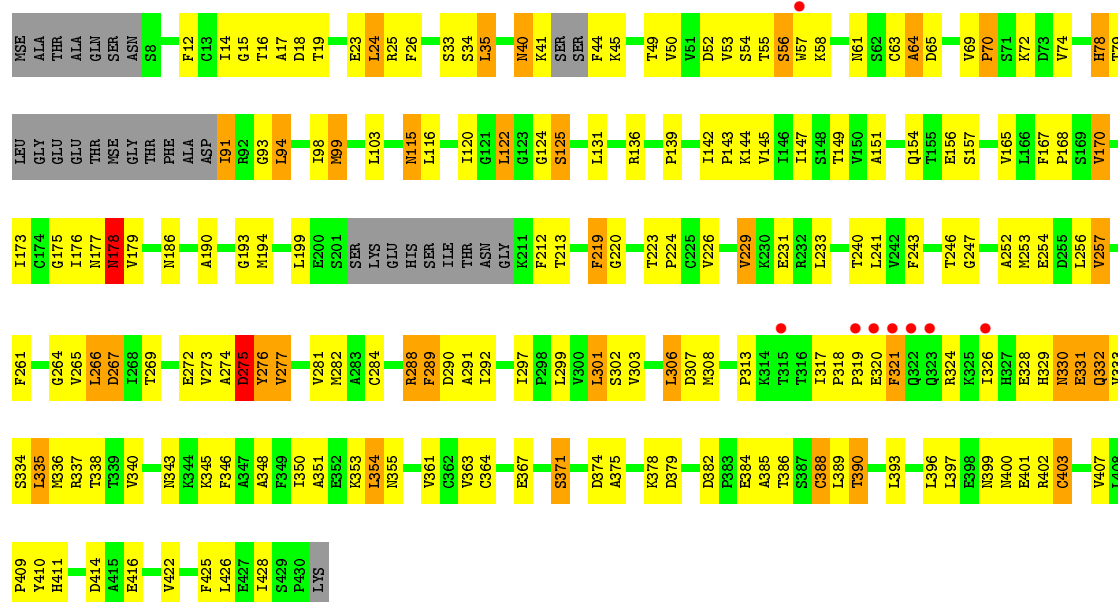




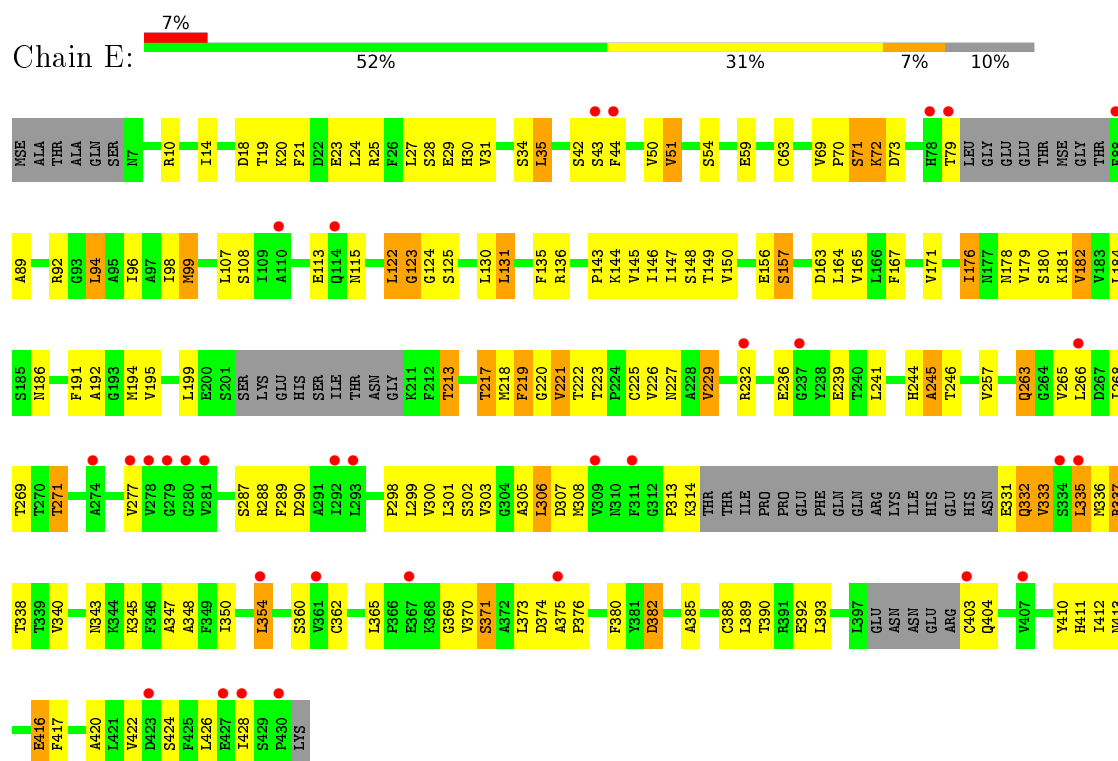
● Molecule 1: Tm-1 protein



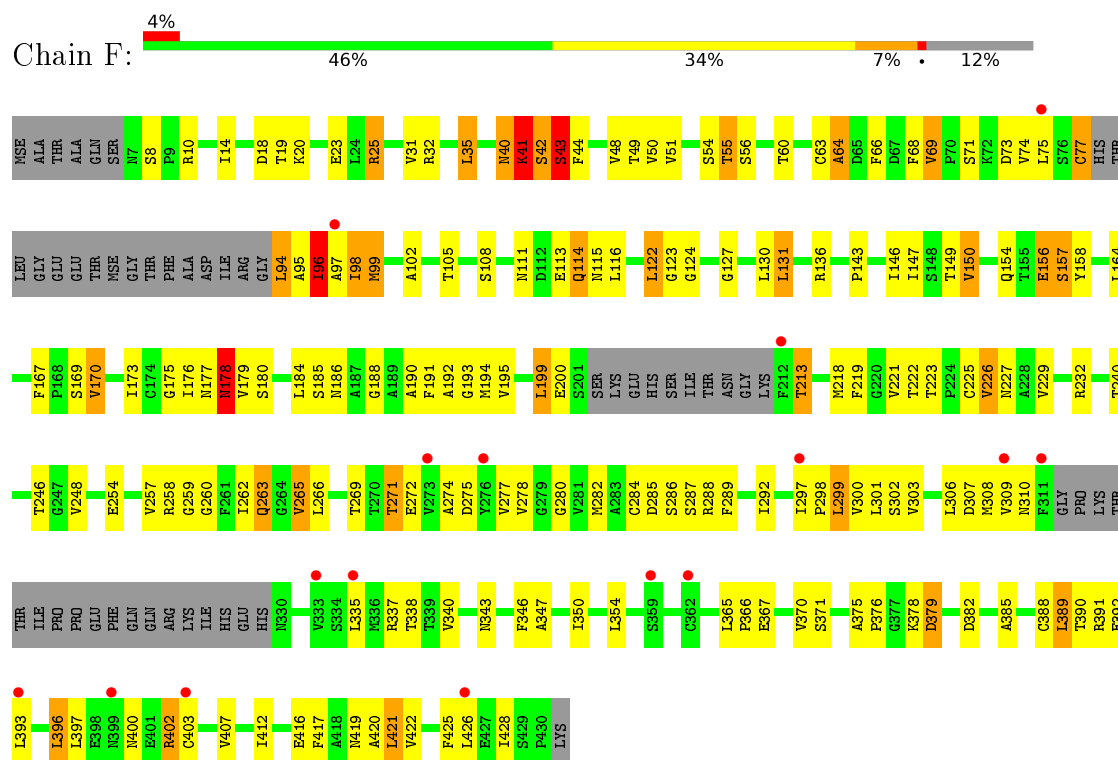
● Molecule 1: Tm-1 protein



• Molecule 1: Tm-1 protein



• Molecule 1: Tm-1 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.97Å 105.28Å 110.62Å 94.56° 109.27° 107.99°	Depositor
Resolution (Å)	49.64 – 2.71 49.64 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.64-2.71) 88.7 (49.64-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.207 , 0.278 0.213 , 0.279	Depositor DCC
$R_{free}$ test set	3975 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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 [i](#)

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

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

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	0.64	0/3088	0.76	0/4167
1	B	0.61	1/3070 (0.0%)	0.73	0/4143
1	C	0.64	1/3034 (0.0%)	0.75	0/4094
1	D	0.67	1/3054 (0.0%)	0.81	0/4120
1	E	0.63	0/2918	0.71	0/3934
1	F	0.57	0/2867	0.71	0/3868
All	All	0.63	3/18031 (0.0%)	0.75	0/24326

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	B	0	2
1	E	0	1
1	F	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	TRP	CD2-CE2	5.69	1.48	1.41
1	D	57	TRP	CD2-CE2	5.46	1.47	1.41
1	C	57	TRP	CD2-CE2	5.12	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	41	LYS	Peptide
1	B	44	PHE	Peptide
1	E	123	GLY	Peptide
1	F	41	LYS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3045	0	3067	147	1
1	B	3027	0	3039	159	0
1	C	2996	0	3013	192	0
1	D	3015	0	3038	161	1
1	E	2881	0	2907	162	0
1	F	2835	0	2850	184	0
2	A	10	0	4	2	0
2	B	10	0	4	0	0
3	A	7	0	0	0	0
3	B	5	0	0	0	0
3	C	12	0	0	1	0
3	D	7	0	0	0	0
3	E	8	0	0	1	0
3	F	5	0	0	0	0
All	All	17863	0	17922	978	1

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 27.

All (978) 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:F:180:SER:O	1:F:184:LEU:HD23	1.42	1.18
1:D:246:THR:HG23	1:D:282:MSE:HE2	1.19	1.11
1:E:143:PRO:HB3	1:E:194:MSE:HE2	1.38	1.02
1:E:191:PHE:O	1:E:195:VAL:HG23	1.62	1.00
1:B:221:VAL:HG21	1:B:308:MSE:HE1	1.43	0.97
1:A:225:CYS:O	1:A:229:VAL:HG23	1.65	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HG21	1:A:308:MSE:HE1	1.47	0.95
1:B:18:ASP:OD1	1:B:19:THR:HG22	1.66	0.95
1:E:269:THR:HG22	1:E:271:THR:HG22	1.47	0.94
1:C:343:ASN:HB3	1:C:389:LEU:HD13	1.49	0.94
1:A:321:PHE:CD1	1:A:336:MSE:HE1	2.03	0.93
1:C:355:ASN:ND2	1:C:400:ASN:HD22	1.67	0.93
1:E:307:ASP:OD2	1:E:370:VAL:HG23	1.69	0.93
1:D:18:ASP:OD1	1:D:19:THR:OG1	1.85	0.92
1:C:355:ASN:HD22	1:C:400:ASN:ND2	1.67	0.91
1:E:147:ILE:N	1:E:147:ILE:HD12	1.83	0.91
1:A:18:ASP:OD2	1:A:54:SER:OG	1.90	0.90
1:A:308:MSE:SE	1:A:335:LEU:HD13	2.22	0.90
1:A:14:ILE:HG23	1:A:51:VAL:HG22	1.53	0.89
1:E:225:CYS:O	1:E:229:VAL:HG12	1.72	0.88
1:E:94:LEU:HD23	1:E:98:ILE:HD11	1.55	0.88
1:D:24:LEU:HD11	1:D:50:VAL:HG13	1.56	0.87
1:D:340:VAL:HG13	1:D:388:CYS:SG	2.14	0.87
1:A:292:ILE:HG23	1:A:297:ILE:HD11	1.55	0.86
1:E:350:ILE:HG22	1:E:354:LEU:HD22	1.58	0.86
1:A:23:GLU:OE2	1:A:175:GLY:N	2.08	0.85
1:F:35:LEU:HD11	1:F:195:VAL:HG21	1.56	0.85
1:A:305:ALA:HB1	1:A:308:MSE:HE3	1.56	0.85
1:E:24:LEU:HD23	1:E:122:LEU:HD11	1.59	0.85
1:E:229:VAL:HG11	1:E:268:ILE:HD11	1.59	0.85
1:D:24:LEU:HD11	1:D:50:VAL:CG1	2.06	0.85
1:C:155:THR:CG2	1:C:159:ILE:HD12	2.06	0.85
1:E:221:VAL:HG23	1:E:222:THR:HG23	1.57	0.84
1:C:339:THR:HG23	1:C:342:GLU:OE1	1.77	0.84
1:D:124:GLY:HA2	1:D:149:THR:OG1	1.78	0.83
1:F:74:VAL:HG23	1:F:99:MSE:HE1	1.58	0.83
1:C:382:ASP:OD2	1:C:385:ALA:HB2	1.78	0.83
1:E:130:LEU:HD23	1:E:131:LEU:HD13	1.59	0.83
1:D:74:VAL:HG11	1:D:99:MSE:SE	2.29	0.82
1:F:246:THR:HG23	1:F:282:MSE:HE2	1.61	0.82
1:F:74:VAL:CG2	1:F:99:MSE:HE1	2.08	0.82
1:A:115:ASN:H	1:A:115:ASN:HD22	1.28	0.82
1:D:329:HIS:HB3	1:D:333:VAL:HG23	1.60	0.82
1:A:307:ASP:OD1	1:A:370:VAL:HG23	1.79	0.82
1:D:384:GLU:O	1:D:388:CYS:SG	2.38	0.82
1:C:330:ASN:O	1:C:333:VAL:HG12	1.80	0.81
1:F:392:GLU:OE2	1:F:396:LEU:HD12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ALA:HB1	1:E:393:LEU:HD22	1.63	0.81
1:F:307:ASP:OD1	1:F:308:MSE:HE3	1.80	0.81
1:E:333:VAL:O	1:E:335:LEU:HD23	1.79	0.81
1:C:265:VAL:HG11	1:C:292:ILE:HD13	1.63	0.81
1:B:350:ILE:HG22	1:B:354:LEU:HD23	1.63	0.81
1:D:335:LEU:N	1:D:335:LEU:HD23	1.94	0.81
1:B:229:VAL:HG23	1:B:233:LEU:HD23	1.62	0.80
1:F:18:ASP:OD2	1:F:54:SER:OG	1.99	0.80
1:C:363:VAL:HG12	1:C:365:LEU:CD2	2.12	0.80
1:B:177:ASN:HD22	1:B:179:VAL:H	1.29	0.80
1:D:397:LEU:HD22	1:D:403:CYS:SG	2.22	0.79
1:E:24:LEU:HD11	1:E:50:VAL:HG13	1.65	0.79
1:F:192:ALA:O	1:F:195:VAL:HG22	1.82	0.79
1:D:91:ILE:HD12	1:D:91:ILE:N	1.98	0.79
1:E:347:ALA:CB	1:E:393:LEU:HD22	2.13	0.79
1:C:355:ASN:HA	1:C:400:ASN:ND2	1.98	0.78
1:A:35:LEU:HD13	1:A:192:ALA:CB	2.13	0.78
1:F:23:GLU:HA	1:F:176:ILE:HD11	1.65	0.78
1:F:308:MSE:SE	1:F:335:LEU:CD2	2.81	0.78
1:C:326:ILE:CG2	1:C:327:HIS:N	2.47	0.78
1:C:330:ASN:O	1:C:333:VAL:CG1	2.32	0.78
1:E:147:ILE:H	1:E:147:ILE:HD12	1.47	0.77
1:A:91:ILE:N	1:A:91:ILE:HD13	1.98	0.77
1:B:269:THR:HG22	1:B:271:THR:HG22	1.67	0.77
1:B:422:VAL:HG12	1:B:426:LEU:HD23	1.67	0.76
1:C:326:ILE:HG23	1:C:327:HIS:H	1.50	0.76
1:F:269:THR:HG22	1:F:271:THR:HG22	1.67	0.76
1:F:265:VAL:HG22	1:F:299:LEU:HD23	1.67	0.76
1:D:350:ILE:HG22	1:D:354:LEU:HD22	1.68	0.76
1:B:216:VAL:HG13	1:B:268:ILE:HD13	1.67	0.76
1:D:23:GLU:OE2	1:D:175:GLY:CA	2.34	0.76
1:B:223:THR:HA	1:B:226:VAL:HG13	1.67	0.76
1:F:49:THR:O	1:F:49:THR:HG22	1.84	0.76
1:C:363:VAL:HG12	1:C:365:LEU:HD21	1.66	0.75
1:E:213:THR:HG23	1:E:263:GLN:HE22	1.49	0.75
1:B:324:ARG:NH2	1:B:339:THR:HG23	2.01	0.75
1:A:386:THR:O	1:A:390:THR:OG1	2.05	0.75
1:E:99:MSE:HG3	1:E:130:LEU:HD11	1.69	0.75
1:B:51:VAL:HG22	1:B:69:VAL:HG13	1.68	0.75
1:B:18:ASP:OD1	1:B:19:THR:CG2	2.34	0.74
1:F:223:THR:HA	1:F:226:VAL:HG13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:MSE:SE	1:F:335:LEU:HD23	2.36	0.74
1:C:246:THR:HG22	1:C:248:VAL:HG22	1.68	0.74
1:C:155:THR:HG21	1:C:159:ILE:HD12	1.69	0.74
1:F:143:PRO:HB3	1:F:194:MSE:HE2	1.69	0.74
1:A:303:VAL:HG23	1:A:370:VAL:HG12	1.69	0.74
1:B:347:ALA:HA	1:B:393:LEU:HD21	1.70	0.74
1:C:241:LEU:HD12	1:C:262:ILE:HD11	1.68	0.74
1:F:266:LEU:HD13	1:F:300:VAL:HB	1.70	0.73
1:C:343:ASN:ND2	1:C:389:LEU:HD22	2.02	0.73
1:B:374:ASP:OD2	1:B:386:THR:HG21	1.89	0.73
1:B:397:LEU:HD13	1:B:403:CYS:SG	2.28	0.73
1:A:90:ASP:C	1:A:91:ILE:HD13	2.09	0.73
1:D:18:ASP:OD1	1:D:19:THR:N	2.22	0.73
1:E:221:VAL:HG23	1:E:222:THR:CG2	2.19	0.73
1:A:165:VAL:HG21	1:B:167:PHE:CE2	2.24	0.72
1:F:301:LEU:HD23	1:F:302:SER:N	2.03	0.72
1:F:350:ILE:HG22	1:F:354:LEU:HD22	1.70	0.72
1:C:307:ASP:OD1	1:C:370:VAL:HG23	1.90	0.72
1:C:130:LEU:HD23	1:C:130:LEU:C	2.10	0.72
1:A:305:ALA:CB	1:A:308:MSE:HE3	2.20	0.72
1:A:355:ASN:HA	1:A:400:ASN:HD22	1.55	0.72
1:A:371:SER:OG	1:A:373:LEU:N	2.23	0.72
1:A:350:ILE:HG22	1:A:354:LEU:HD23	1.71	0.71
1:C:313:PRO:C	1:C:317:ILE:HG21	2.10	0.71
1:F:51:VAL:HB	1:F:69:VAL:HG13	1.70	0.71
1:F:99:MSE:O	1:F:102:ALA:N	2.23	0.71
1:F:136:ARG:NH1	1:F:158:TYR:O	2.20	0.71
1:E:220:GLY:O	1:E:223:THR:HG23	1.91	0.71
1:F:180:SER:O	1:F:184:LEU:CD2	2.33	0.71
1:C:367:GLU:HG3	1:C:407:VAL:HG12	1.73	0.71
1:F:274:ALA:HB1	1:F:309:VAL:HG22	1.71	0.71
1:B:422:VAL:HG12	1:B:426:LEU:CD2	2.19	0.71
1:C:130:LEU:HD22	1:C:131:LEU:HD13	1.72	0.71
1:F:173:ILE:HG22	1:F:173:ILE:O	1.89	0.71
1:B:24:LEU:HD21	1:B:50:VAL:HG13	1.72	0.70
1:C:397:LEU:HD22	1:C:403:CYS:SG	2.31	0.70
1:B:122:LEU:HD12	1:B:122:LEU:O	1.92	0.70
1:D:23:GLU:OE2	1:D:175:GLY:N	2.24	0.70
1:B:422:VAL:O	1:B:426:LEU:HD23	1.92	0.70
1:E:70:PRO:HD2	1:E:73:ASP:OD2	1.90	0.70
1:A:35:LEU:HD13	1:A:192:ALA:HB1	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:O	1:B:24:LEU:HD23	1.91	0.69
1:F:75:LEU:CD2	1:F:99:MSE:HE3	2.22	0.69
1:D:17:ALA:HB3	1:D:52:ASP:OD2	1.92	0.69
1:F:150:VAL:HG23	1:F:150:VAL:O	1.93	0.69
1:F:343:ASN:ND2	1:F:385:ALA:HB1	2.07	0.69
1:F:41:LYS:N	1:F:42:SER:HB2	2.08	0.69
1:A:301:LEU:HD23	1:A:302:SER:N	2.07	0.69
1:A:301:LEU:HD13	1:A:354:LEU:HD21	1.75	0.69
1:F:113:GLU:O	1:F:115:ASN:N	2.26	0.68
1:A:350:ILE:CG2	1:A:354:LEU:HD23	2.24	0.68
1:B:305:ALA:HB1	1:B:308:MSE:HE3	1.73	0.68
1:A:422:VAL:O	1:A:426:LEU:HD23	1.94	0.68
1:E:180:SER:O	1:E:184:LEU:HD13	1.95	0.67
1:F:25:ARG:HD2	1:F:64:ALA:HB2	1.75	0.67
1:E:422:VAL:O	1:E:426:LEU:HD23	1.94	0.67
1:B:321:PHE:CD1	1:B:336:MSE:HE1	2.30	0.67
1:C:394:GLN:O	1:C:398:GLU:N	2.28	0.67
1:B:422:VAL:O	1:B:426:LEU:CD2	2.42	0.67
1:B:365:LEU:CD1	1:B:390:THR:HG23	2.24	0.67
1:D:220:GLY:O	1:D:223:THR:HG23	1.95	0.67
1:E:226:VAL:O	1:E:229:VAL:HG13	1.95	0.67
1:F:367:GLU:CG	1:F:407:VAL:HG12	2.25	0.67
1:C:246:THR:HG22	1:C:246:THR:O	1.94	0.66
1:C:258:ARG:NH2	1:C:291:ALA:HB2	2.10	0.66
1:F:347:ALA:HB1	1:F:393:LEU:CD2	2.26	0.66
1:C:308:MSE:SE	1:C:335:LEU:HD12	2.46	0.66
1:F:254:GLU:HA	1:F:257:VAL:HG13	1.78	0.66
1:C:274:ALA:O	1:C:275:ASP:C	2.34	0.66
1:E:266:LEU:HD13	1:E:300:VAL:HB	1.77	0.66
1:A:422:VAL:HG12	1:A:426:LEU:HD23	1.77	0.65
1:C:179:VAL:HG21	1:D:256:LEU:HD13	1.78	0.65
1:C:18:ASP:OD1	1:C:19:THR:N	2.30	0.65
1:E:360:SER:HB2	1:E:428:ILE:HG23	1.78	0.65
1:E:337:ARG:NH2	1:E:374:ASP:OD2	2.29	0.65
1:A:219:PHE:HB2	1:A:269:THR:HG21	1.79	0.65
1:C:320:GLU:N	1:C:320:GLU:OE1	2.30	0.65
1:E:362:CYS:HB2	1:E:428:ILE:HD11	1.78	0.65
1:C:240:THR:O	1:C:240:THR:HG22	1.97	0.65
1:E:371:SER:O	1:E:411:HIS:CE1	2.50	0.65
1:C:350:ILE:HG22	1:C:354:LEU:HD22	1.79	0.65
1:D:53:VAL:HA	1:D:99:MSE:HE3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:VAL:HG23	1:E:227:ASN:HD22	1.62	0.65
1:D:308:MSE:SE	1:D:335:LEU:HD12	2.48	0.64
1:E:350:ILE:CG2	1:E:354:LEU:HD22	2.27	0.64
1:B:365:LEU:HD13	1:B:390:THR:HG23	1.78	0.64
1:E:124:GLY:HA2	1:E:149:THR:OG1	1.98	0.64
1:B:225:CYS:O	1:B:229:VAL:CG1	2.45	0.64
1:E:226:VAL:CG2	1:E:227:ASN:N	2.60	0.64
1:F:272:GLU:HB3	1:F:284:CYS:HB3	1.80	0.64
1:D:145:VAL:HG22	1:D:165:VAL:CG1	2.27	0.64
1:F:266:LEU:HD21	1:F:425:PHE:CD2	2.33	0.64
1:D:351:ALA:CB	1:D:396:LEU:HD13	2.27	0.64
1:D:422:VAL:O	1:D:426:LEU:HD23	1.98	0.64
1:E:194:MSE:HE3	1:F:186:ASN:HB3	1.80	0.64
1:B:266:LEU:HD11	1:B:425:PHE:CD2	2.32	0.63
1:B:284:CYS:HB2	1:B:288:ARG:HG2	1.80	0.63
1:D:24:LEU:CD1	1:D:50:VAL:CG1	2.75	0.63
1:B:28:SER:OG	1:B:50:VAL:HG22	1.99	0.63
1:F:122:LEU:H	1:F:122:LEU:HD12	1.62	0.63
1:D:124:GLY:O	1:D:125:SER:C	2.37	0.63
1:B:365:LEU:HD13	1:B:390:THR:HA	1.79	0.63
1:F:23:GLU:HG3	1:F:176:ILE:HD13	1.81	0.63
1:D:290:ASP:OD1	1:D:353:LYS:NZ	2.31	0.63
1:D:74:VAL:CG1	1:D:99:MSE:SE	2.96	0.63
1:F:246:THR:O	1:F:246:THR:HG22	1.97	0.63
1:A:394:GLN:HB3	1:A:405:VAL:HG11	1.80	0.63
1:C:363:VAL:CG1	1:C:365:LEU:HD21	2.28	0.63
1:F:99:MSE:O	1:F:102:ALA:HB3	1.99	0.63
1:F:275:ASP:HA	1:F:309:VAL:HG13	1.80	0.63
1:A:246:THR:HG23	1:A:282:MSE:SE	2.49	0.63
1:C:343:ASN:HA	1:C:346:PHE:CD2	2.34	0.63
1:E:130:LEU:CD2	1:E:131:LEU:HD13	2.28	0.63
1:B:350:ILE:HG22	1:B:354:LEU:CD2	2.29	0.62
1:C:263:GLN:O	1:C:297:ILE:HB	1.99	0.62
1:F:94:LEU:HD22	1:F:97:ALA:HB3	1.79	0.62
1:A:94:LEU:CD2	1:A:98:ILE:HD11	2.29	0.62
1:D:25:ARG:HD2	1:D:64:ALA:HB2	1.81	0.62
1:B:143:PRO:HB3	1:B:194:MSE:HE2	1.79	0.62
1:D:317:ILE:HG23	1:D:318:PRO:HD2	1.80	0.62
1:E:219:PHE:HB3	1:E:221:VAL:HG22	1.80	0.62
1:E:222:THR:HA	1:E:413:ASN:HD21	1.65	0.62
1:D:63:CYS:O	1:D:64:ALA:C	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LEU:O	1:C:357:ALA:HB2	1.99	0.62
1:E:360:SER:CB	1:E:428:ILE:HG23	2.28	0.62
1:E:94:LEU:CD2	1:E:98:ILE:HD11	2.28	0.62
1:F:35:LEU:HD11	1:F:195:VAL:CG2	2.29	0.62
1:D:144:LYS:O	1:D:165:VAL:HG12	1.98	0.62
1:D:264:GLY:HA2	1:D:297:ILE:HD12	1.82	0.62
1:F:63:CYS:O	1:F:64:ALA:C	2.38	0.62
1:B:266:LEU:O	1:B:268:ILE:HD12	2.00	0.62
1:A:31:VAL:HG12	1:A:35:LEU:HD22	1.81	0.61
1:A:332:GLN:HA	1:A:332:GLN:HE21	1.65	0.61
1:C:328:GLU:OE1	1:C:330:ASN:N	2.34	0.61
1:F:298:PRO:HB3	1:F:428:ILE:HG22	1.80	0.61
1:F:232:ARG:HG3	1:F:422:VAL:HG11	1.81	0.61
1:A:303:VAL:HG23	1:A:370:VAL:CG1	2.31	0.61
1:C:194:MSE:HE3	1:D:186:ASN:HB3	1.81	0.61
1:E:226:VAL:HG23	1:E:227:ASN:N	2.13	0.61
1:B:254:GLU:HA	1:B:257:VAL:HG13	1.83	0.61
1:D:18:ASP:OD2	1:D:54:SER:OG	2.18	0.61
1:E:333:VAL:O	1:E:335:LEU:CD2	2.49	0.61
1:E:225:CYS:O	1:E:229:VAL:CG1	2.47	0.60
1:B:257:VAL:HG22	1:B:258:ARG:N	2.16	0.60
1:C:325:LYS:O	1:C:326:ILE:HG13	2.02	0.60
1:B:225:CYS:O	1:B:229:VAL:HG12	2.01	0.60
1:B:301:LEU:HD23	1:B:302:SER:N	2.16	0.60
1:C:335:LEU:N	1:C:335:LEU:HD23	2.15	0.60
1:E:171:VAL:HG13	1:E:179:VAL:HG11	1.84	0.60
1:F:32:ARG:HB2	1:F:48:VAL:HG21	1.82	0.60
1:D:147:ILE:H	1:D:147:ILE:HD12	1.65	0.60
1:D:308:MSE:SE	1:D:335:LEU:CD1	2.99	0.60
1:E:375:ALA:HB2	1:E:411:HIS:NE2	2.17	0.60
1:E:143:PRO:HB3	1:E:194:MSE:CE	2.21	0.60
1:B:217:THR:CG2	1:B:253:MSE:HE1	2.32	0.60
1:B:371:SER:O	1:B:374:ASP:N	2.35	0.60
1:B:121:GLY:O	1:B:146:ILE:HA	2.02	0.60
1:B:308:MSE:SE	1:B:335:LEU:HD13	2.51	0.60
1:B:355:ASN:HA	1:B:400:ASN:HD22	1.66	0.59
1:B:176:ILE:HG23	1:B:181:LYS:HG3	1.83	0.59
1:D:335:LEU:CD2	1:D:335:LEU:N	2.65	0.59
1:E:213:THR:HG23	1:E:263:GLN:NE2	2.16	0.59
1:C:337:ARG:HG2	1:C:380:PHE:HB3	1.85	0.59
1:C:275:ASP:O	1:C:279:GLY:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LYS:HA	1:C:317:ILE:HD13	1.83	0.59
1:D:266:LEU:HD21	1:D:425:PHE:CD1	2.38	0.59
1:F:262:ILE:HG22	1:F:262:ILE:O	2.02	0.59
1:F:275:ASP:O	1:F:280:GLY:N	2.31	0.59
1:E:18:ASP:OD2	1:E:54:SER:OG	2.20	0.59
1:F:246:THR:HB	1:F:248:VAL:HG22	1.85	0.59
1:B:269:THR:HA	1:B:304:GLY:HA3	1.85	0.59
1:F:226:VAL:O	1:F:229:VAL:HG22	2.03	0.59
1:E:218:MSE:HG3	1:E:226:VAL:HG11	1.84	0.59
1:E:229:VAL:HG11	1:E:268:ILE:CD1	2.33	0.59
1:A:272:GLU:HB3	1:A:284:CYS:HB3	1.85	0.58
1:F:340:VAL:HG13	1:F:385:ALA:HA	1.85	0.58
1:D:124:GLY:CA	1:D:149:THR:OG1	2.49	0.58
1:E:221:VAL:HG21	1:E:308:MSE:CE	2.33	0.58
1:D:23:GLU:OE2	1:D:175:GLY:HA2	2.03	0.58
1:F:154:GLN:OE1	1:F:156:GLU:HB3	2.02	0.58
1:A:113:GLU:HB2	1:A:115:ASN:ND2	2.19	0.58
1:B:232:ARG:HG2	1:B:422:VAL:HG11	1.85	0.58
1:E:144:LYS:HB3	1:E:164:LEU:HD12	1.85	0.58
1:E:221:VAL:HG21	1:E:308:MSE:HE1	1.86	0.58
1:E:365:LEU:HD13	1:E:390:THR:HG23	1.84	0.58
1:A:354:LEU:HD12	1:A:361:VAL:HG11	1.84	0.58
1:D:266:LEU:HD21	1:D:425:PHE:CG	2.39	0.58
1:F:195:VAL:O	1:F:199:LEU:HD22	2.03	0.58
1:D:375:ALA:HB3	1:D:378:LYS:HG3	1.86	0.58
1:A:211:LYS:O	1:A:212:PHE:C	2.41	0.58
1:E:347:ALA:CB	1:E:393:LEU:CD2	2.82	0.58
1:C:149:THR:CG2	1:C:173:ILE:HD12	2.34	0.58
1:F:232:ARG:CG	1:F:422:VAL:HG11	2.34	0.58
1:B:177:ASN:O	1:B:179:VAL:N	2.37	0.57
1:F:303:VAL:HG23	1:F:370:VAL:CG1	2.34	0.57
1:B:177:ASN:ND2	1:B:179:VAL:H	2.00	0.57
1:B:229:VAL:HG23	1:B:233:LEU:CD2	2.34	0.57
1:D:139:PRO:HD2	1:D:142:ILE:HD12	1.86	0.57
1:A:292:ILE:HG23	1:A:297:ILE:CD1	2.30	0.57
1:C:219:PHE:HB2	1:C:269:THR:HG21	1.86	0.57
1:C:343:ASN:CB	1:C:389:LEU:HD13	2.30	0.57
1:B:122:LEU:HD12	1:B:122:LEU:C	2.25	0.57
1:E:219:PHE:O	1:E:220:GLY:C	2.43	0.57
1:F:366:PRO:HG2	1:F:370:VAL:HG12	1.86	0.57
1:C:326:ILE:HG22	1:C:327:HIS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:SER:OG	1:B:303:VAL:N	2.37	0.57
1:B:321:PHE:HB2	1:B:324:ARG:HG3	1.86	0.57
1:D:301:LEU:C	1:D:301:LEU:HD23	2.24	0.57
1:E:298:PRO:HB3	1:E:428:ILE:HG22	1.86	0.57
1:F:40:ASN:C	1:F:42:SER:HB2	2.25	0.57
1:F:143:PRO:CB	1:F:194:MSE:HE2	2.35	0.57
1:A:363:VAL:HG12	1:A:364:CYS:N	2.19	0.57
1:B:143:PRO:HG2	1:B:195:VAL:HG22	1.87	0.57
1:E:71:SER:O	1:E:72:LYS:C	2.41	0.57
1:B:275:ASP:HA	1:B:309:VAL:HG22	1.86	0.57
1:C:186:ASN:HB3	1:D:194:MSE:HE3	1.87	0.57
1:F:343:ASN:HA	1:F:346:PHE:CD2	2.40	0.57
1:C:259:GLY:O	1:C:261:PHE:CD1	2.58	0.56
1:C:271:THR:HB	1:C:305:ALA:HB3	1.87	0.56
1:E:18:ASP:OD1	1:E:19:THR:N	2.38	0.56
1:A:303:VAL:CG2	1:A:370:VAL:HG12	2.34	0.56
1:A:330:ASN:O	1:A:332:GLN:N	2.37	0.56
1:E:34:SER:O	1:E:35:LEU:C	2.43	0.56
1:F:350:ILE:O	1:F:354:LEU:HD13	2.05	0.56
1:F:55:THR:HG21	1:F:95:ALA:HB1	1.86	0.56
1:C:179:VAL:HG22	1:D:261:PHE:CD2	2.41	0.56
1:C:273:VAL:CG1	1:C:273:VAL:O	2.53	0.56
1:C:264:GLY:HA2	1:C:297:ILE:HD12	1.87	0.56
1:E:147:ILE:N	1:E:147:ILE:CD1	2.59	0.56
1:F:277:VAL:HG21	1:F:346:PHE:HE1	1.70	0.56
1:C:240:THR:CG2	1:C:240:THR:O	2.53	0.56
1:B:122:LEU:CD1	1:B:122:LEU:C	2.73	0.56
1:B:31:VAL:HG12	1:B:35:LEU:HD22	1.87	0.56
1:D:53:VAL:HG11	1:D:103:LEU:HD22	1.88	0.56
1:F:8:SER:HB2	1:F:44:PHE:CD1	2.40	0.56
1:C:246:THR:CG2	1:C:246:THR:O	2.54	0.56
1:C:355:ASN:HA	1:C:400:ASN:HD21	1.67	0.56
1:E:289:PHE:CE1	1:E:301:LEU:HD11	2.41	0.56
1:D:302:SER:OG	1:D:303:VAL:N	2.39	0.56
1:D:91:ILE:CD1	1:D:91:ILE:N	2.67	0.56
1:F:347:ALA:HB1	1:F:393:LEU:HD23	1.87	0.56
1:C:363:VAL:HG12	1:C:365:LEU:HD22	1.87	0.56
1:D:343:ASN:HB3	1:D:389:LEU:HD13	1.88	0.56
1:E:14:ILE:HG12	1:E:51:VAL:HG13	1.86	0.56
1:C:38:PHE:O	1:C:40:ASN:N	2.39	0.56
1:C:32:ARG:HB2	1:C:48:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:MSE:HB2	1:A:226:VAL:HG11	1.88	0.55
1:A:360:SER:HB2	1:A:428:ILE:HG23	1.88	0.55
1:B:150:VAL:O	1:B:150:VAL:HG23	2.06	0.55
1:C:386:THR:O	1:C:390:THR:OG1	2.19	0.55
1:B:216:VAL:CG1	1:B:268:ILE:HD13	2.36	0.55
1:A:94:LEU:HD21	1:A:98:ILE:HD11	1.87	0.55
1:A:165:VAL:HG21	1:B:167:PHE:CD2	2.40	0.55
1:C:381:TYR:O	1:C:382:ASP:CB	2.55	0.55
1:A:327:HIS:CD2	1:A:373:LEU:HD11	2.42	0.55
1:D:343:ASN:HA	1:D:346:PHE:CD2	2.42	0.55
1:F:23:GLU:OE2	1:F:175:GLY:N	2.30	0.55
1:F:96:ILE:HG22	1:F:97:ALA:N	2.21	0.55
1:B:303:VAL:CB	1:B:306:LEU:HD23	2.36	0.55
1:C:389:LEU:O	1:C:393:LEU:HD23	2.06	0.55
1:A:343:ASN:HD22	1:A:389:LEU:HD22	1.71	0.55
1:B:42:SER:OG	1:B:43:SER:N	2.38	0.55
1:C:23:GLU:OE2	1:C:175:GLY:N	2.36	0.55
1:C:327:HIS:CD2	1:C:327:HIS:O	2.59	0.55
1:E:371:SER:O	1:E:411:HIS:NE2	2.39	0.55
1:A:90:ASP:O	1:A:92:ARG:N	2.39	0.55
1:D:14:ILE:HG22	1:D:15:GLY:N	2.21	0.55
1:E:217:THR:HG22	1:E:245:ALA:HB2	1.88	0.55
1:D:411:HIS:HB3	1:D:414:ASP:OD2	2.07	0.55
1:C:307:ASP:O	1:C:308:MSE:HE2	2.06	0.55
1:F:402:ARG:NE	1:F:402:ARG:HA	2.22	0.55
1:A:221:VAL:CG2	1:A:308:MSE:HE1	2.30	0.54
1:D:25:ARG:HG3	1:D:63:CYS:SG	2.47	0.54
1:E:18:ASP:CG	1:E:54:SER:OG	2.45	0.54
1:E:232:ARG:HG3	1:E:422:VAL:HG11	1.89	0.54
1:F:31:VAL:O	1:F:35:LEU:HD22	2.07	0.54
1:C:266:LEU:HD13	1:C:300:VAL:HB	1.88	0.54
1:C:273:VAL:HG12	1:C:273:VAL:O	2.08	0.54
1:C:347:ALA:CB	1:C:393:LEU:HD22	2.38	0.54
1:C:337:ARG:CG	1:C:380:PHE:HB3	2.37	0.54
1:D:49:THR:HG22	1:D:50:VAL:N	2.22	0.54
1:F:74:VAL:HG23	1:F:99:MSE:CE	2.33	0.54
1:C:374:ASP:OD2	1:C:386:THR:HG21	2.07	0.54
1:D:40:ASN:O	1:D:40:ASN:ND2	2.39	0.54
1:E:308:MSE:SE	1:E:335:LEU:HD12	2.57	0.54
1:E:362:CYS:CB	1:E:428:ILE:HD11	2.36	0.54
1:F:343:ASN:HB3	1:F:389:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:VAL:HA	1:B:306:LEU:CD2	2.37	0.54
1:B:417:PHE:CE2	1:B:421:LEU:HD11	2.43	0.54
1:C:367:GLU:CG	1:C:407:VAL:HG12	2.37	0.54
1:E:145:VAL:HG13	1:E:167:PHE:CD1	2.43	0.54
1:A:94:LEU:HD22	1:A:94:LEU:O	2.08	0.54
1:C:278:VAL:O	1:C:278:VAL:HG12	2.08	0.54
1:F:191:PHE:O	1:F:195:VAL:HG13	2.08	0.54
1:C:221:VAL:CG2	1:C:371:SER:OG	2.56	0.54
1:A:324:ARG:CZ	1:A:339:THR:HG23	2.38	0.54
1:E:218:MSE:CG	1:E:226:VAL:HG11	2.37	0.54
1:F:40:ASN:OD1	1:F:40:ASN:C	2.46	0.54
1:A:371:SER:HG	1:A:373:LEU:H	1.56	0.53
1:C:275:ASP:HB3	1:C:283:ALA:HB2	1.90	0.53
1:D:24:LEU:CD1	1:D:50:VAL:HG11	2.38	0.53
1:E:35:LEU:HD13	1:E:192:ALA:CB	2.38	0.53
1:C:410:TYR:CE1	1:C:416:GLU:HG3	2.43	0.53
1:E:332:GLN:O	1:E:333:VAL:C	2.46	0.53
1:C:274:ALA:O	1:C:276:TYR:N	2.41	0.53
1:C:96:ILE:HG22	1:C:97:ALA:N	2.22	0.53
1:D:289:PHE:O	1:D:292:ILE:N	2.37	0.53
1:E:186:ASN:HB3	1:F:194:MSE:HE3	1.90	0.53
1:A:324:ARG:NH2	1:A:339:THR:HG23	2.24	0.53
1:B:217:THR:HG21	1:B:253:MSE:HE1	1.91	0.53
1:C:28:SER:O	1:C:29:GLU:C	2.47	0.53
1:D:340:VAL:HG22	1:D:385:ALA:HA	1.90	0.53
1:F:177:ASN:O	1:F:179:VAL:N	2.42	0.53
1:A:23:GLU:OE2	1:A:175:GLY:CA	2.57	0.53
1:A:363:VAL:CG1	1:A:364:CYS:N	2.71	0.53
1:B:24:LEU:C	1:B:24:LEU:HD23	2.28	0.53
1:B:258:ARG:NH2	1:B:291:ALA:HB2	2.23	0.53
1:B:25:ARG:HD2	1:B:64:ALA:HB2	1.91	0.53
1:C:337:ARG:HD2	1:C:338:THR:O	2.08	0.53
1:C:17:ALA:HB3	1:C:52:ASP:OD2	2.08	0.53
1:E:35:LEU:HD13	1:E:192:ALA:HB1	1.91	0.53
1:C:285:ASP:OD1	1:C:285:ASP:C	2.46	0.53
1:C:37:SER:O	1:C:40:ASN:HB2	2.08	0.53
1:C:69:VAL:HG22	1:C:69:VAL:O	2.08	0.53
1:D:193:GLY:O	1:D:194:MSE:C	2.46	0.53
1:E:350:ILE:HG22	1:E:354:LEU:CD2	2.36	0.53
1:B:246:THR:O	1:B:246:THR:HG22	2.07	0.53
1:C:154:GLN:HB2	1:D:154:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ILE:HG23	1:F:51:VAL:HG22	1.91	0.53
1:A:417:PHE:O	1:A:420:ALA:HB3	2.09	0.52
1:D:53:VAL:C	1:D:99:MSE:HE3	2.29	0.52
1:D:63:CYS:O	1:D:65:ASP:N	2.42	0.52
1:D:334:SER:C	1:D:335:LEU:HD23	2.30	0.52
1:D:290:ASP:OD1	1:D:353:LYS:HD2	2.09	0.52
1:E:14:ILE:HG12	1:E:51:VAL:CG1	2.38	0.52
1:F:20:LYS:HA	1:F:23:GLU:OE1	2.09	0.52
1:C:373:LEU:N	1:C:373:LEU:HD12	2.24	0.52
1:C:149:THR:HA	1:C:169:SER:OG	2.09	0.52
1:D:301:LEU:HD22	1:D:363:VAL:HG22	1.89	0.52
1:E:269:THR:CG2	1:E:271:THR:HG22	2.29	0.52
1:B:35:LEU:HD13	1:B:192:ALA:CB	2.40	0.52
1:B:361:VAL:HG12	1:B:362:CYS:N	2.24	0.52
1:F:186:ASN:HD22	1:F:186:ASN:N	2.07	0.52
1:A:20:LYS:HG2	1:A:173:ILE:HG22	1.92	0.52
1:D:177:ASN:O	1:D:178:ASN:C	2.47	0.52
1:D:53:VAL:CA	1:D:99:MSE:HE3	2.39	0.52
1:A:257:VAL:HG12	1:A:262:ILE:CG2	2.39	0.52
1:B:417:PHE:O	1:B:420:ALA:HB3	2.09	0.52
1:C:106:PHE:CD1	1:C:106:PHE:C	2.82	0.52
1:D:246:THR:HG22	1:D:246:THR:O	2.09	0.52
1:D:317:ILE:HG22	1:D:318:PRO:O	2.09	0.52
1:F:35:LEU:CD1	1:F:195:VAL:CG2	2.87	0.52
1:D:319:PRO:O	1:D:321:PHE:N	2.43	0.52
1:E:30:HIS:O	1:E:30:HIS:CG	2.63	0.52
1:E:343:ASN:O	1:E:389:LEU:HD13	2.09	0.52
1:F:74:VAL:HG21	1:F:99:MSE:SE	2.60	0.52
1:D:229:VAL:HG23	1:D:233:LEU:HD12	1.92	0.51
1:D:345:LYS:O	1:D:348:ALA:N	2.42	0.51
1:D:273:VAL:O	1:D:277:VAL:HG23	2.09	0.51
1:C:254:GLU:OE2	1:C:289:PHE:N	2.36	0.51
1:D:115:ASN:N	1:D:115:ASN:OD1	2.43	0.51
1:D:34:SER:O	1:D:35:LEU:C	2.48	0.51
1:E:347:ALA:HB2	1:E:393:LEU:CD2	2.40	0.51
1:C:277:VAL:CG2	1:C:278:VAL:HG23	2.40	0.51
1:E:136:ARG:NH1	1:E:157:SER:O	2.44	0.51
1:E:221:VAL:CG2	1:E:222:THR:HG23	2.34	0.51
1:F:375:ALA:HB3	1:F:378:LYS:HG3	1.93	0.51
1:C:214:VAL:CG1	1:C:266:LEU:HD23	2.41	0.51
1:C:51:VAL:HG23	1:C:52:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:LEU:O	1:F:338:THR:HG21	2.09	0.51
1:B:226:VAL:HA	1:B:229:VAL:HG13	1.91	0.51
1:B:375:ALA:HB3	1:B:378:LYS:HG3	1.92	0.51
1:F:75:LEU:HD23	1:F:99:MSE:HE3	1.93	0.51
1:A:115:ASN:H	1:A:115:ASN:ND2	2.03	0.51
1:A:213:THR:CG2	1:A:241:LEU:HD12	2.41	0.51
1:A:355:ASN:HA	1:A:400:ASN:ND2	2.23	0.51
1:B:13:CYS:HA	1:B:120:ILE:HG23	1.93	0.51
1:C:130:LEU:HD23	1:C:130:LEU:O	2.10	0.51
1:C:327:HIS:O	1:C:328:GLU:C	2.49	0.51
1:C:221:VAL:HG21	1:C:371:SER:OG	2.10	0.51
1:D:350:ILE:HG22	1:D:354:LEU:CD2	2.36	0.51
1:D:382:ASP:OD1	1:D:382:ASP:C	2.49	0.51
1:D:386:THR:O	1:D:390:THR:OG1	2.26	0.51
1:F:307:ASP:OD2	1:F:370:VAL:HG23	2.11	0.51
1:B:147:ILE:HD12	1:B:147:ILE:H	1.74	0.51
1:E:371:SER:OG	1:E:373:LEU:N	2.44	0.51
1:F:122:LEU:N	1:F:122:LEU:HD12	2.26	0.51
1:B:258:ARG:HH21	1:B:291:ALA:HB2	1.76	0.50
1:C:381:TYR:O	1:C:382:ASP:HB2	2.11	0.50
1:A:213:THR:HG21	1:A:241:LEU:HD12	1.92	0.50
1:F:299:LEU:C	1:F:299:LEU:HD22	2.31	0.50
1:B:196:ILE:HG22	1:B:197:GLY:N	2.25	0.50
1:C:365:LEU:HD22	1:C:365:LEU:N	2.27	0.50
1:D:243:PHE:CE1	1:D:253:MSE:HG3	2.45	0.50
1:F:35:LEU:CD1	1:F:195:VAL:HG21	2.35	0.50
1:A:221:VAL:HG23	1:A:221:VAL:O	2.11	0.50
1:C:343:ASN:HD22	1:C:389:LEU:HD22	1.74	0.50
1:C:194:MSE:CG	1:D:190:ALA:HB2	2.41	0.50
1:E:24:LEU:CD1	1:E:50:VAL:HG13	2.39	0.50
1:F:367:GLU:HG3	1:F:407:VAL:HG12	1.92	0.50
1:B:216:VAL:HG13	1:B:268:ILE:CD1	2.40	0.50
1:B:59:GLU:HG2	1:B:61:ASN:HD21	1.76	0.50
1:C:369:GLY:HA3	1:C:374:ASP:O	2.11	0.50
1:D:122:LEU:CD1	1:D:122:LEU:C	2.80	0.50
1:D:400:ASN:OD1	1:D:402:ARG:HB2	2.11	0.50
1:A:34:SER:O	1:A:35:LEU:C	2.48	0.50
1:D:143:PRO:HB3	1:D:194:MSE:HE2	1.94	0.50
1:F:350:ILE:O	1:F:354:LEU:N	2.44	0.50
1:A:360:SER:CB	1:A:428:ILE:HG23	2.42	0.50
1:B:94:LEU:HD13	1:B:94:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:THR:HG21	1:D:151:ALA:O	2.12	0.50
1:C:334:SER:C	1:C:335:LEU:HD23	2.32	0.50
1:A:214:VAL:HG12	1:A:215:GLY:N	2.27	0.50
1:A:257:VAL:HG12	1:A:262:ILE:HG22	1.94	0.50
1:C:28:SER:OG	1:C:50:VAL:HG22	2.11	0.50
1:E:411:HIS:CE1	1:E:412:ILE:HG22	2.47	0.50
1:B:354:LEU:O	1:B:357:ALA:HB2	2.12	0.49
1:D:136:ARG:NH1	1:D:157:SER:O	2.41	0.49
1:D:145:VAL:HG13	1:D:165:VAL:HG13	1.94	0.49
1:A:284:CYS:HB2	1:A:288:ARG:CG	2.42	0.49
1:B:268:ILE:O	1:B:304:GLY:HA3	2.11	0.49
1:C:155:THR:HG23	1:C:159:ILE:HD12	1.93	0.49
1:C:10:ARG:NH1	1:C:49:THR:OG1	2.40	0.49
1:E:226:VAL:CG2	1:E:227:ASN:H	2.25	0.49
1:F:123:GLY:HA2	1:F:173:ILE:HD13	1.94	0.49
1:B:299:LEU:C	1:B:299:LEU:HD22	2.32	0.49
1:D:274:ALA:O	1:D:276:TYR:N	2.45	0.49
1:D:94:LEU:O	1:D:94:LEU:HD22	2.11	0.49
1:E:412:ILE:HG23	1:E:413:ASN:N	2.27	0.49
1:B:265:VAL:HG22	1:B:299:LEU:HD23	1.94	0.49
1:F:51:VAL:CB	1:F:69:VAL:HG13	2.40	0.49
1:A:418:ALA:O	1:A:422:VAL:HG23	2.12	0.49
1:D:253:MSE:O	1:D:257:VAL:HG13	2.12	0.49
1:D:24:LEU:CD1	1:D:50:VAL:HG13	2.36	0.49
1:E:410:TYR:CE1	1:E:416:GLU:HG3	2.48	0.49
1:E:96:ILE:HG23	1:E:130:LEU:HB2	1.94	0.49
1:A:360:SER:O	1:A:361:VAL:HG23	2.12	0.49
1:A:229:VAL:HG13	1:A:422:VAL:HG22	1.93	0.49
1:E:195:VAL:O	1:E:199:LEU:HD13	2.13	0.49
1:E:25:ARG:HG3	1:E:63:CYS:SG	2.53	0.49
1:C:130:LEU:CD2	1:C:130:LEU:C	2.81	0.49
1:C:223:THR:O	1:C:224:PRO:C	2.44	0.49
1:C:235:LYS:NZ	1:C:235:LYS:HB2	2.28	0.49
1:C:299:LEU:CD2	1:C:299:LEU:C	2.81	0.49
1:F:32:ARG:CB	1:F:48:VAL:HG21	2.42	0.49
1:F:71:SER:HA	1:F:74:VAL:HG22	1.95	0.49
1:B:169:SER:C	1:B:170:VAL:HG23	2.32	0.49
1:B:232:ARG:CG	1:B:422:VAL:HG11	2.43	0.49
1:C:336:MSE:O	1:C:337:ARG:C	2.51	0.49
1:D:177:ASN:ND2	1:D:179:VAL:H	2.10	0.49
1:F:275:ASP:HA	1:F:309:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:VAL:CG2	1:F:99:MSE:CE	2.88	0.49
1:C:245:ALA:HB1	1:C:272:GLU:HG3	1.95	0.48
1:F:347:ALA:HA	1:F:393:LEU:HD21	1.94	0.48
1:F:99:MSE:O	1:F:102:ALA:CB	2.61	0.48
1:B:373:LEU:HB3	1:B:380:PHE:HB2	1.95	0.48
1:D:351:ALA:HB1	1:D:396:LEU:HB3	1.95	0.48
1:F:420:ALA:O	1:F:421:LEU:C	2.52	0.48
1:A:69:VAL:O	1:A:69:VAL:HG22	2.11	0.48
1:B:219:PHE:HB2	1:B:269:THR:HG21	1.95	0.48
1:B:360:SER:HB2	1:B:428:ILE:HG23	1.95	0.48
1:C:329:HIS:O	1:C:330:ASN:CG	2.52	0.48
1:E:31:VAL:HG12	1:E:35:LEU:CD2	2.44	0.48
1:F:274:ALA:CB	1:F:309:VAL:HG22	2.42	0.48
1:B:131:LEU:O	1:B:132:SER:C	2.52	0.48
1:E:410:TYR:CD1	1:E:416:GLU:HG3	2.48	0.48
1:F:412:ILE:HA	1:F:417:PHE:CD2	2.48	0.48
1:F:69:VAL:HG23	1:F:73:ASP:HB2	1.94	0.48
1:A:122:LEU:H	1:A:122:LEU:HD12	1.77	0.48
1:A:249:GLY:O	1:A:252:ALA:HB3	2.14	0.48
1:A:266:LEU:HD21	1:A:425:PHE:CG	2.49	0.48
1:B:18:ASP:CG	1:B:19:THR:HG22	2.31	0.48
1:D:284:CYS:HB2	1:D:288:ARG:HG2	1.94	0.48
1:C:119:VAL:O	1:C:119:VAL:HG23	2.13	0.48
1:A:35:LEU:CD1	1:A:192:ALA:HB1	2.41	0.48
1:B:14:ILE:O	1:B:121:GLY:HA2	2.14	0.48
1:E:303:VAL:CA	1:E:306:LEU:HD22	2.44	0.48
1:C:249:GLY:O	1:C:250:GLY:C	2.52	0.48
1:D:363:VAL:CG1	1:D:364:CYS:N	2.77	0.48
1:D:374:ASP:OD2	1:D:386:THR:HG21	2.14	0.48
1:D:18:ASP:CG	1:D:54:SER:HG	2.15	0.48
1:A:171:VAL:HG23	1:A:172:ASP:O	2.14	0.48
1:A:266:LEU:HD13	1:A:300:VAL:HB	1.94	0.48
1:B:69:VAL:HG23	1:B:73:ASP:HB2	1.95	0.48
1:C:30:HIS:HB2	3:C:508:HOH:O	2.13	0.48
1:C:54:SER:O	1:C:99:MSE:HE3	2.14	0.48
1:D:122:LEU:HD12	1:D:122:LEU:O	2.14	0.48
1:A:220:GLY:O	1:A:223:THR:HG23	2.14	0.48
1:A:285:ASP:OD1	1:A:285:ASP:C	2.52	0.48
1:B:225:CYS:O	1:B:229:VAL:HG13	2.12	0.48
1:B:257:VAL:CG2	1:B:258:ARG:N	2.77	0.48
1:B:351:ALA:HA	1:B:397:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:VAL:O	1:B:69:VAL:HG22	2.12	0.48
1:C:113:GLU:N	1:C:113:GLU:OE1	2.47	0.48
1:C:417:PHE:O	1:C:420:ALA:HB3	2.13	0.48
1:D:17:ALA:CB	1:D:52:ASP:CG	2.82	0.48
1:F:169:SER:O	1:F:170:VAL:HB	2.13	0.48
1:F:51:VAL:HA	1:F:69:VAL:HG13	1.95	0.48
1:B:265:VAL:HG11	1:B:292:ILE:CD1	2.44	0.47
1:C:69:VAL:CG2	1:C:69:VAL:O	2.62	0.47
1:D:281:VAL:O	1:D:281:VAL:HG12	2.14	0.47
1:E:220:GLY:O	1:E:222:THR:N	2.47	0.47
1:A:281:VAL:HG13	1:A:282:MSE:HG3	1.96	0.47
1:D:17:ALA:CB	1:D:52:ASP:OD2	2.61	0.47
1:E:122:LEU:H	1:E:122:LEU:HD12	1.79	0.47
1:F:18:ASP:OD1	1:F:19:THR:N	2.46	0.47
1:C:261:PHE:CD2	1:D:179:VAL:HG22	2.49	0.47
1:C:373:LEU:N	1:C:373:LEU:CD1	2.78	0.47
1:D:307:ASP:OD2	1:D:371:SER:HB3	2.14	0.47
1:A:145:VAL:HG12	1:A:146:ILE:N	2.30	0.47
1:B:35:LEU:HD13	1:B:192:ALA:HB1	1.96	0.47
1:C:143:PRO:HB3	1:C:194:MSE:HE2	1.97	0.47
1:C:196:ILE:O	1:C:197:GLY:C	2.53	0.47
1:C:384:GLU:HG2	1:C:385:ALA:N	2.29	0.47
1:D:428:ILE:CG2	1:D:428:ILE:O	2.63	0.47
1:E:145:VAL:HG13	1:E:167:PHE:CE1	2.49	0.47
1:E:232:ARG:O	1:E:236:GLU:HB2	2.14	0.47
1:E:369:GLY:HA3	1:E:374:ASP:O	2.14	0.47
1:E:417:PHE:O	1:E:420:ALA:HB3	2.13	0.47
1:F:123:GLY:HA2	1:F:173:ILE:CD1	2.45	0.47
1:F:254:GLU:OE2	1:F:289:PHE:N	2.48	0.47
1:C:109:ILE:O	1:C:109:ILE:CG2	2.62	0.47
1:C:109:ILE:HG22	1:C:109:ILE:O	2.15	0.47
1:C:190:ALA:HB2	1:D:194:MSE:HG2	1.96	0.47
1:D:176:ILE:N	1:D:176:ILE:HD13	2.29	0.47
1:A:71:SER:O	1:A:72:LYS:C	2.52	0.47
1:B:214:VAL:HG12	1:B:215:GLY:N	2.30	0.47
1:C:290:ASP:CG	1:C:353:LYS:HZ3	2.18	0.47
1:A:90:ASP:CA	1:A:91:ILE:HD13	2.44	0.47
1:B:303:VAL:O	1:B:304:GLY:C	2.53	0.47
1:C:257:VAL:HG12	1:C:262:ILE:CG2	2.45	0.47
1:C:34:SER:O	1:C:35:LEU:C	2.53	0.47
1:E:239:GLU:OE2	1:F:177:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:LEU:HD23	1:E:302:SER:N	2.30	0.47
1:F:10:ARG:NH1	1:F:49:THR:OG1	2.47	0.47
1:F:343:ASN:HD21	1:F:385:ALA:HB1	1.79	0.47
1:F:32:ARG:NH1	1:F:66:PHE:CE1	2.83	0.47
1:A:35:LEU:HA	1:A:35:LEU:HD12	1.84	0.47
1:B:229:VAL:O	1:B:233:LEU:HD23	2.15	0.47
1:C:284:CYS:HB2	1:C:288:ARG:HG2	1.97	0.47
1:D:23:GLU:HG2	1:D:173:ILE:HG23	1.96	0.47
1:F:292:ILE:HG23	1:F:297:ILE:CD1	2.45	0.47
1:C:190:ALA:HB2	1:D:194:MSE:CG	2.45	0.46
1:D:177:ASN:O	1:D:179:VAL:N	2.48	0.46
1:E:147:ILE:H	1:E:147:ILE:CD1	2.20	0.46
1:F:136:ARG:NH1	1:F:157:SER:O	2.46	0.46
1:F:258:ARG:C	1:F:260:GLY:H	2.18	0.46
1:B:306:LEU:O	1:B:338:THR:HG21	2.16	0.46
1:B:321:PHE:CG	1:B:336:MSE:HE1	2.50	0.46
1:E:122:LEU:HD12	1:E:122:LEU:N	2.31	0.46
1:E:340:VAL:HG13	1:E:385:ALA:HA	1.97	0.46
1:F:301:LEU:C	1:F:301:LEU:HD23	2.36	0.46
1:B:417:PHE:O	1:B:420:ALA:N	2.47	0.46
1:C:347:ALA:HB1	1:C:393:LEU:HD22	1.97	0.46
1:E:287:SER:HA	1:E:290:ASP:OD2	2.16	0.46
1:F:99:MSE:HE2	1:F:102:ALA:HB3	1.96	0.46
1:A:226:VAL:CG2	1:A:227:ASN:N	2.79	0.46
1:A:410:TYR:CE1	1:A:416:GLU:HG3	2.50	0.46
1:B:327:HIS:O	1:B:327:HIS:ND1	2.48	0.46
1:C:306:LEU:HD12	1:C:306:LEU:HA	1.81	0.46
1:E:345:LYS:O	1:E:348:ALA:HB3	2.16	0.46
1:C:22:ASP:O	1:C:176:ILE:HD11	2.15	0.46
1:C:19:THR:HG22	1:C:19:THR:O	2.14	0.46
1:E:305:ALA:CB	1:E:308:MSE:HE3	2.45	0.46
1:B:303:VAL:CA	1:B:306:LEU:HD23	2.45	0.46
1:E:150:VAL:HG23	1:E:150:VAL:O	2.16	0.46
1:F:392:GLU:OE2	1:F:396:LEU:CD1	2.55	0.46
1:D:26:PHE:CD1	1:D:26:PHE:C	2.89	0.46
1:D:264:GLY:CA	1:D:297:ILE:HD12	2.44	0.46
1:E:123:GLY:O	1:E:148:SER:HA	2.16	0.46
1:E:31:VAL:O	1:E:35:LEU:HD22	2.15	0.46
1:A:321:PHE:CE1	1:A:336:MSE:HE1	2.50	0.46
1:A:347:ALA:CB	1:A:393:LEU:HD22	2.46	0.46
1:C:39:SER:HB2	1:C:196:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:VAL:HG21	1:D:167:PHE:CE2	2.50	0.46
1:D:219:PHE:HB2	1:D:269:THR:HG21	1.97	0.46
1:D:94:LEU:HD22	1:D:98:ILE:HG13	1.96	0.46
1:E:403:CYS:SG	1:E:404:GLN:N	2.88	0.46
1:A:262:ILE:HG22	1:A:262:ILE:O	2.16	0.46
1:B:361:VAL:CG1	1:B:362:CYS:N	2.78	0.46
1:D:94:LEU:HD22	1:D:98:ILE:CD1	2.46	0.46
1:E:178:ASN:O	1:E:182:VAL:HG12	2.16	0.46
1:E:226:VAL:HA	1:E:229:VAL:HG13	1.98	0.46
1:F:347:ALA:CB	1:F:392:GLU:HG3	2.45	0.46
1:A:343:ASN:ND2	1:A:389:LEU:HD22	2.31	0.46
1:B:303:VAL:HB	1:B:306:LEU:HD23	1.98	0.46
1:C:256:LEU:HD13	1:D:179:VAL:HG21	1.98	0.46
1:C:277:VAL:CG2	1:C:278:VAL:N	2.78	0.46
1:C:335:LEU:CD2	1:C:335:LEU:N	2.79	0.46
1:A:186:ASN:HB3	1:B:194:MSE:HE3	1.97	0.45
1:B:221:VAL:CG2	1:B:308:MSE:HE1	2.30	0.45
1:D:17:ALA:HB2	1:D:52:ASP:CG	2.36	0.45
1:B:388:CYS:O	1:B:392:GLU:HB2	2.16	0.45
1:C:308:MSE:SE	1:C:335:LEU:CD1	3.14	0.45
1:C:391:ARG:O	1:C:392:GLU:C	2.55	0.45
1:C:9:PRO:HG2	1:C:46:VAL:HG22	1.98	0.45
1:E:94:LEU:HD23	1:E:98:ILE:CD1	2.38	0.45
1:F:419:ASN:O	1:F:420:ALA:C	2.53	0.45
1:A:25:ARG:HG3	1:A:63:CYS:SG	2.56	0.45
1:D:306:LEU:HD12	1:D:306:LEU:HA	1.68	0.45
1:E:347:ALA:HB3	1:E:392:GLU:HG2	1.99	0.45
1:B:255:ASP:OD1	1:B:258:ARG:NH1	2.44	0.45
1:B:278:VAL:HG23	1:B:278:VAL:O	2.15	0.45
1:A:218:MSE:CB	1:A:226:VAL:HG11	2.46	0.45
1:A:248:VAL:HG23	1:A:249:GLY:H	1.82	0.45
1:A:271:THR:O	1:A:274:ALA:HB3	2.17	0.45
1:A:365:LEU:HD13	1:A:390:THR:HG23	1.99	0.45
1:B:12:PHE:O	1:B:120:ILE:HG22	2.17	0.45
1:C:259:GLY:O	1:C:261:PHE:CE1	2.70	0.45
1:F:69:VAL:O	1:F:69:VAL:HG22	2.17	0.45
1:E:226:VAL:O	1:E:229:VAL:N	2.48	0.45
1:F:225:CYS:O	1:F:229:VAL:HG13	2.17	0.45
1:A:354:LEU:CD1	1:A:361:VAL:HG11	2.47	0.45
1:C:115:ASN:N	1:C:115:ASN:OD1	2.50	0.45
1:C:140:ILE:HG22	1:C:141:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:PRO:O	1:C:320:GLU:C	2.55	0.45
1:C:337:ARG:CD	1:C:338:THR:O	2.65	0.45
1:E:373:LEU:HB3	1:E:380:PHE:HB2	1.99	0.45
1:E:165:VAL:HG21	1:F:167:PHE:CE2	2.52	0.45
1:C:106:PHE:CD1	1:C:106:PHE:O	2.69	0.45
1:F:350:ILE:HG23	1:F:354:LEU:CD1	2.46	0.45
1:A:422:VAL:HG12	1:A:426:LEU:CD2	2.46	0.45
1:B:422:VAL:O	1:B:426:LEU:HD22	2.15	0.45
1:C:107:LEU:HD13	1:C:138:LEU:HD11	1.98	0.45
1:C:293:LEU:O	1:C:296:LYS:N	2.47	0.45
1:F:223:THR:HA	1:F:226:VAL:CG1	2.44	0.45
1:F:246:THR:HG23	1:F:282:MSE:CE	2.42	0.45
1:F:350:ILE:HG23	1:F:354:LEU:HD13	1.98	0.45
1:F:390:THR:HG21	1:F:407:VAL:HG13	1.98	0.45
1:A:269:THR:HA	1:A:304:GLY:HA3	1.98	0.44
1:D:247:GLY:N	1:D:272:GLU:OE2	2.35	0.44
1:D:321:PHE:CD1	1:D:336:MSE:HE1	2.52	0.44
1:F:23:GLU:HG3	1:F:176:ILE:CD1	2.46	0.44
1:B:422:VAL:CG1	1:B:426:LEU:CD2	2.94	0.44
1:D:363:VAL:HG12	1:D:364:CYS:N	2.31	0.44
1:A:139:PRO:HB2	1:A:142:ILE:HD12	1.98	0.44
1:C:130:LEU:CD2	1:C:131:LEU:HD13	2.45	0.44
1:C:223:THR:HA	1:C:226:VAL:HG13	1.98	0.44
1:D:361:VAL:O	1:D:403:CYS:HA	2.18	0.44
1:E:213:THR:HG21	1:F:178:ASN:OD1	2.18	0.44
1:A:18:ASP:OD1	1:A:19:THR:N	2.51	0.44
2:A:501:TLA:O1	2:A:501:TLA:O3	2.34	0.44
1:C:176:ILE:HG23	1:C:181:LYS:HG3	1.98	0.44
1:C:230:LYS:HE3	1:C:240:THR:HG21	1.99	0.44
1:C:94:LEU:HD13	1:C:94:LEU:C	2.38	0.44
1:E:115:ASN:N	1:E:115:ASN:OD1	2.48	0.44
1:E:300:VAL:HA	1:E:362:CYS:O	2.17	0.44
1:E:303:VAL:HA	1:E:306:LEU:HD22	1.99	0.44
1:F:391:ARG:O	1:F:392:GLU:C	2.55	0.44
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.79	0.44
1:A:60:THR:HG22	1:A:68:PHE:CZ	2.52	0.44
1:D:410:TYR:CE1	1:D:416:GLU:HG3	2.53	0.44
1:A:9:PRO:HG3	1:A:199:LEU:HD21	1.99	0.44
1:D:330:ASN:O	1:D:331:GLU:C	2.56	0.44
1:D:321:PHE:CE1	1:D:336:MSE:HE1	2.53	0.44
1:E:24:LEU:HD23	1:E:122:LEU:CD1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:ASP:CG	1:F:309:VAL:HG13	2.37	0.44
1:F:347:ALA:HB3	1:F:392:GLU:HG3	2.00	0.44
1:F:41:LYS:CA	1:F:42:SER:CB	2.95	0.44
1:A:367:GLU:HG3	1:A:407:VAL:HG12	2.00	0.44
1:B:124:GLY:HA2	1:B:149:THR:OG1	2.18	0.44
1:B:182:VAL:CG2	1:B:183:VAL:N	2.81	0.44
1:B:274:ALA:O	1:B:278:VAL:HG13	2.17	0.44
1:B:426:LEU:HA	1:B:426:LEU:HD13	1.91	0.44
1:C:313:PRO:HB3	1:C:332:GLN:HA	2.00	0.44
1:E:298:PRO:HB3	1:E:428:ILE:CG2	2.47	0.44
1:A:142:ILE:O	1:A:144:LYS:HG3	2.18	0.44
1:A:290:ASP:OD2	1:A:353:LYS:NZ	2.51	0.44
1:B:23:GLU:N	1:B:23:GLU:OE1	2.51	0.44
1:B:303:VAL:HA	1:B:306:LEU:HD23	1.98	0.44
1:C:411:HIS:HE1	1:C:413:ASN:HD22	1.65	0.44
1:D:124:GLY:O	1:D:125:SER:O	2.35	0.44
1:D:274:ALA:O	1:D:275:ASP:C	2.56	0.44
1:D:343:ASN:HB3	1:D:389:LEU:CD1	2.48	0.44
1:E:31:VAL:CG1	1:E:35:LEU:CD2	2.96	0.44
1:F:292:ILE:HG23	1:F:297:ILE:HD11	1.99	0.44
1:F:98:ILE:O	1:F:98:ILE:HD13	2.18	0.44
1:A:265:VAL:HG11	1:A:292:ILE:HD13	1.99	0.44
1:A:90:ASP:N	1:A:90:ASP:OD1	2.50	0.44
1:C:149:THR:HG23	1:C:173:ILE:HD12	2.00	0.44
1:E:287:SER:CA	1:E:290:ASP:OD2	2.66	0.44
1:E:42:SER:O	1:E:44:PHE:N	2.51	0.44
1:D:40:ASN:HA	1:D:41:LYS:HA	1.78	0.43
1:D:16:THR:HG22	1:D:54:SER:HA	1.99	0.43
1:E:360:SER:HB3	1:E:428:ILE:HG23	1.98	0.43
1:F:146:ILE:HG22	1:F:147:ILE:O	2.18	0.43
1:E:24:LEU:O	1:E:24:LEU:HD13	2.18	0.43
1:E:27:LEU:O	1:E:28:SER:C	2.56	0.43
1:F:63:CYS:HB2	1:F:68:PHE:CD2	2.54	0.43
1:A:79:THR:HG23	1:A:105:THR:HG21	2.01	0.43
1:A:216:VAL:HG11	1:A:226:VAL:HB	2.00	0.43
1:B:419:ASN:O	1:B:423:ASP:CG	2.57	0.43
1:B:75:LEU:HA	1:B:75:LEU:HD23	1.85	0.43
1:D:149:THR:HG23	1:D:173:ILE:HD12	2.00	0.43
1:E:21:PHE:N	3:E:507:HOH:O	2.52	0.43
1:F:25:ARG:HG3	1:F:63:CYS:SG	2.59	0.43
1:F:274:ALA:HB1	1:F:309:VAL:CG2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ASP:O	1:F:287:SER:N	2.50	0.43
1:A:40:ASN:HA	1:A:41:LYS:HA	1.82	0.43
1:A:362:CYS:SG	1:A:424:SER:HB3	2.57	0.43
1:A:17:ALA:N	1:A:52:ASP:OD1	2.44	0.43
1:C:371:SER:O	1:C:411:HIS:NE2	2.51	0.43
1:D:12:PHE:CE1	1:D:116:LEU:HD12	2.53	0.43
1:E:221:VAL:HG11	1:E:308:MSE:HE1	2.01	0.43
1:E:24:LEU:CD1	1:E:50:VAL:CG1	2.96	0.43
1:F:226:VAL:HG22	1:F:227:ASN:N	2.33	0.43
1:F:258:ARG:C	1:F:260:GLY:N	2.71	0.43
1:F:299:LEU:HD22	1:F:300:VAL:N	2.34	0.43
1:F:50:VAL:O	1:F:69:VAL:HG12	2.19	0.43
1:D:329:HIS:HB3	1:D:333:VAL:CG2	2.41	0.43
1:A:163:ASP:OD1	1:A:163:ASP:N	2.50	0.43
1:A:24:LEU:HD13	1:A:50:VAL:HG13	1.99	0.43
1:B:270:THR:OG1	1:B:306:LEU:HD21	2.18	0.43
1:C:154:GLN:HB2	1:D:154:GLN:NE2	2.33	0.43
1:C:374:ASP:OD2	1:C:386:THR:CG2	2.65	0.43
1:E:307:ASP:HA	1:E:338:THR:OG1	2.19	0.43
1:F:277:VAL:HG23	1:F:278:VAL:HG23	2.00	0.43
1:F:365:LEU:HD13	1:F:390:THR:CG2	2.49	0.43
1:A:194:MSE:HE3	1:B:186:ASN:HB3	2.01	0.43
1:A:309:VAL:HG12	1:A:311:PHE:CE2	2.53	0.43
1:C:345:LYS:O	1:C:348:ALA:HB3	2.18	0.43
1:E:178:ASN:ND2	1:F:213:THR:HG23	2.34	0.43
1:F:14:ILE:HG12	1:F:51:VAL:HG13	2.01	0.43
1:C:12:PHE:CE1	1:C:49:THR:HG21	2.54	0.43
1:C:347:ALA:O	1:C:351:ALA:CB	2.67	0.43
1:E:163:ASP:OD1	1:E:163:ASP:N	2.52	0.43
1:E:176:ILE:HG23	1:E:181:LYS:HG3	2.00	0.43
1:F:185:SER:O	1:F:188:GLY:N	2.46	0.43
1:A:168:PRO:HG2	1:B:163:ASP:HA	1.99	0.43
1:B:277:VAL:CG2	1:B:346:PHE:HE1	2.31	0.43
1:C:140:ILE:CD1	1:D:170:VAL:HG11	2.49	0.43
1:C:417:PHE:O	1:C:418:ALA:C	2.57	0.43
1:D:289:PHE:O	1:D:290:ASP:C	2.57	0.43
1:D:308:MSE:SE	1:D:335:LEU:HD13	2.69	0.43
1:D:371:SER:O	1:D:411:HIS:NE2	2.52	0.43
1:E:244:HIS:O	1:E:246:THR:OG1	2.26	0.43
1:F:218:MSE:CG	1:F:226:VAL:HG11	2.48	0.43
1:A:284:CYS:HB2	1:A:288:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:PRO:HA	1:A:386:THR:OG1	2.18	0.43
1:B:228:ALA:O	1:B:231:GLU:HB2	2.19	0.43
1:C:355:ASN:HA	1:C:400:ASN:HD22	1.79	0.43
1:E:135:PHE:HD2	1:E:164:LEU:HD11	1.83	0.43
1:F:111:ASN:HD22	1:F:116:LEU:HB3	1.84	0.43
1:F:307:ASP:OD1	1:F:308:MSE:CE	2.61	0.43
1:A:159:ILE:O	1:A:162:SER:OG	2.30	0.42
1:A:350:ILE:HG23	1:A:354:LEU:HD23	2.01	0.42
1:C:313:PRO:O	1:C:317:ILE:HG21	2.19	0.42
1:D:145:VAL:HG22	1:D:165:VAL:HG11	1.98	0.42
1:D:306:LEU:O	1:D:338:THR:HG21	2.18	0.42
1:D:355:ASN:HA	1:D:400:ASN:ND2	2.33	0.42
1:E:24:LEU:HD11	1:E:50:VAL:CG1	2.43	0.42
1:F:150:VAL:HG21	1:F:158:TYR:OH	2.18	0.42
1:F:74:VAL:CB	1:F:99:MSE:HE1	2.49	0.42
1:B:314:LYS:HG3	1:B:315:THR:N	2.34	0.42
1:D:120:ILE:HD11	1:D:147:ILE:HD11	2.02	0.42
1:B:219:PHE:O	1:B:220:GLY:C	2.58	0.42
1:D:147:ILE:HD12	1:D:147:ILE:N	2.34	0.42
1:D:14:ILE:CG2	1:D:15:GLY:N	2.82	0.42
1:F:298:PRO:HB3	1:F:428:ILE:CG2	2.46	0.42
1:A:408:LEU:HD11	1:A:420:ALA:HB1	2.01	0.42
1:A:232:ARG:HG3	1:A:422:VAL:HG11	2.01	0.42
1:C:253:MSE:O	1:C:257:VAL:HG13	2.20	0.42
1:C:96:ILE:CG2	1:C:97:ALA:N	2.83	0.42
1:F:292:ILE:HG21	1:F:299:LEU:HG	2.01	0.42
1:D:12:PHE:HE1	1:D:116:LEU:HD12	1.84	0.42
1:F:111:ASN:O	1:F:114:GLN:HA	2.20	0.42
1:A:284:CYS:HB2	1:A:288:ARG:HG3	2.00	0.42
1:B:232:ARG:NE	1:B:236:GLU:OE2	2.46	0.42
1:B:369:GLY:HA2	1:B:374:ASP:OD2	2.20	0.42
1:D:382:ASP:OD2	1:D:385:ALA:HB2	2.19	0.42
1:E:14:ILE:HD13	1:E:51:VAL:HG11	2.01	0.42
1:F:131:LEU:HD12	1:F:131:LEU:HA	1.91	0.42
1:F:303:VAL:HB	1:F:306:LEU:HD12	2.00	0.42
1:F:365:LEU:HD13	1:F:390:THR:HG23	2.01	0.42
1:A:367:GLU:CG	1:A:407:VAL:HG12	2.50	0.42
1:B:285:ASP:OD1	1:B:287:SER:OG	2.35	0.42
1:B:363:VAL:CG1	1:B:364:CYS:N	2.82	0.42
1:B:53:VAL:HA	1:B:99:MSE:HE3	2.02	0.42
1:D:355:ASN:HD22	1:D:400:ASN:HD22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:PRO:O	1:D:410:TYR:CD1	2.73	0.42
1:D:78:HIS:HA	1:D:79:THR:HA	1.74	0.42
1:F:365:LEU:HB3	1:F:390:THR:HG23	2.02	0.42
1:F:42:SER:OG	1:F:43:SER:N	2.49	0.42
1:A:31:VAL:CG1	1:A:35:LEU:HD22	2.48	0.42
1:A:374:ASP:OD2	1:A:386:THR:HG21	2.20	0.42
1:C:142:ILE:O	1:C:144:LYS:HG3	2.19	0.42
1:C:214:VAL:HG11	1:C:266:LEU:HD23	2.01	0.42
1:E:223:THR:HA	1:E:226:VAL:HG22	2.01	0.42
1:E:263:GLN:N	1:E:263:GLN:HE21	2.18	0.42
1:C:404:GLN:CB	1:F:43:SER:O	2.68	0.42
1:A:31:VAL:HG12	1:A:35:LEU:CD2	2.48	0.42
1:B:265:VAL:HG11	1:B:292:ILE:HD13	2.01	0.42
1:B:63:CYS:HB2	1:B:68:PHE:CD2	2.55	0.42
1:C:307:ASP:OD1	1:C:370:VAL:CG2	2.65	0.42
1:C:326:ILE:CG2	1:C:327:HIS:H	2.11	0.42
1:E:107:LEU:O	1:E:108:SER:C	2.58	0.42
1:E:350:ILE:O	1:E:354:LEU:HB2	2.20	0.42
1:A:122:LEU:N	1:A:122:LEU:HD12	2.35	0.41
1:B:107:LEU:HD13	1:B:119:VAL:HG11	2.01	0.41
1:B:146:ILE:HD12	1:B:164:LEU:HD21	2.02	0.41
1:E:300:VAL:HG22	1:E:362:CYS:HB3	2.02	0.41
1:E:422:VAL:HG12	1:E:426:LEU:HD23	2.02	0.41
1:F:258:ARG:O	1:F:260:GLY:N	2.53	0.41
1:A:312:GLY:HA3	1:A:332:GLN:O	2.20	0.41
1:A:66:PHE:CD1	2:A:501:TLA:O41	2.74	0.41
1:B:178:ASN:HB3	1:B:179:VAL:HG23	2.01	0.41
1:C:306:LEU:O	1:C:308:MSE:N	2.51	0.41
1:F:124:GLY:CA	1:F:149:THR:OG1	2.68	0.41
1:A:253:MSE:O	1:A:257:VAL:HG13	2.20	0.41
1:A:375:ALA:O	1:A:377:GLY:N	2.53	0.41
1:A:241:LEU:HD21	1:B:177:ASN:ND2	2.35	0.41
1:B:214:VAL:HG11	1:B:266:LEU:CD1	2.50	0.41
1:C:317:ILE:O	1:C:318:PRO:O	2.38	0.41
1:C:327:HIS:HD2	1:C:327:HIS:O	2.01	0.41
1:D:351:ALA:HB3	1:D:396:LEU:HD13	2.02	0.41
1:F:347:ALA:CA	1:F:393:LEU:HD21	2.50	0.41
1:B:365:LEU:HD12	1:B:390:THR:HG23	2.00	0.41
1:C:278:VAL:O	1:C:278:VAL:CG1	2.67	0.41
1:C:390:THR:H	1:C:390:THR:HG1	1.44	0.41
1:E:371:SER:N	1:E:412:ILE:HG21	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ILE:CG1	1:E:51:VAL:HG13	2.48	0.41
1:E:241:LEU:HD21	1:F:177:ASN:ND2	2.36	0.41
1:F:277:VAL:CG2	1:F:278:VAL:N	2.83	0.41
1:F:69:VAL:HG23	1:F:73:ASP:CB	2.51	0.41
1:F:74:VAL:O	1:F:77:CYS:SG	2.78	0.41
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.75	0.41
1:B:343:ASN:HA	1:B:346:PHE:CD2	2.56	0.41
1:B:58:LYS:HD3	1:B:59:GLU:N	2.35	0.41
1:C:63:CYS:O	1:C:64:ALA:C	2.58	0.41
1:D:177:ASN:HD22	1:D:179:VAL:H	1.68	0.41
1:E:130:LEU:HD23	1:E:131:LEU:N	2.36	0.41
1:E:226:VAL:HG22	1:E:227:ASN:H	1.85	0.41
1:F:303:VAL:CG2	1:F:370:VAL:CG1	2.98	0.41
1:B:306:LEU:HA	1:B:306:LEU:HD13	1.91	0.41
1:B:305:ALA:CB	1:B:308:MSE:HE3	2.47	0.41
1:D:252:ALA:O	1:D:256:LEU:HG	2.21	0.41
1:D:35:LEU:HD12	1:D:35:LEU:HA	1.77	0.41
1:F:382:ASP:OD2	1:F:385:ALA:HB2	2.21	0.41
1:E:382:ASP:OD2	1:E:385:ALA:HB2	2.20	0.41
1:A:35:LEU:CD1	1:A:192:ALA:CB	2.94	0.41
1:A:303:VAL:CG2	1:A:370:VAL:CG1	2.97	0.41
1:A:354:LEU:HD13	1:A:354:LEU:HA	1.82	0.41
1:B:340:VAL:HG21	1:B:384:GLU:OE2	2.21	0.41
1:C:382:ASP:OD2	1:C:385:ALA:CB	2.59	0.41
1:D:223:THR:N	1:D:224:PRO:CD	2.84	0.41
1:F:275:ASP:CA	1:F:309:VAL:HG13	2.50	0.41
1:F:307:ASP:OD2	1:F:371:SER:HB3	2.21	0.41
1:F:365:LEU:HD12	1:F:407:VAL:HG22	2.01	0.41
1:F:41:LYS:HA	1:F:42:SER:CB	2.50	0.41
1:C:271:THR:HB	1:C:305:ALA:CB	2.49	0.41
1:D:253:MSE:HE1	1:D:267:ASP:OD2	2.21	0.41
1:D:326:ILE:HD13	1:D:336:MSE:HA	2.03	0.41
1:F:277:VAL:CG2	1:F:278:VAL:HG23	2.51	0.41
1:F:397:LEU:CD2	1:F:400:ASN:HD22	2.34	0.41
1:A:99:MSE:O	1:A:102:ALA:HB3	2.21	0.41
1:B:112:ASP:C	1:B:114:GLN:N	2.75	0.41
1:B:177:ASN:HD21	1:B:179:VAL:HB	1.85	0.41
1:B:70:PRO:HD2	1:B:73:ASP:OD2	2.21	0.41
1:D:69:VAL:HG23	1:D:70:PRO:N	2.36	0.41
1:B:131:LEU:O	1:B:134:ALA:N	2.55	0.40
1:B:375:ALA:HB3	1:B:378:LYS:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:HD12	1:C:262:ILE:CD1	2.43	0.40
1:C:354:LEU:HA	1:C:354:LEU:HD12	1.92	0.40
1:C:35:LEU:HD12	1:C:35:LEU:HA	1.95	0.40
1:C:409:PRO:O	1:C:410:TYR:CD1	2.74	0.40
1:D:254:GLU:OE1	1:D:291:ALA:HB3	2.21	0.40
1:D:367:GLU:HG3	1:D:407:VAL:HG12	2.03	0.40
1:E:42:SER:C	1:E:44:PHE:H	2.25	0.40
1:B:307:ASP:OD1	1:B:308:MSE:HE2	2.22	0.40
1:B:404:GLN:CG	1:B:405:VAL:N	2.84	0.40
1:B:390:THR:CG2	1:B:407:VAL:HG22	2.52	0.40
1:F:303:VAL:HG23	1:F:370:VAL:HG12	2.03	0.40
1:A:113:GLU:CB	1:A:115:ASN:ND2	2.84	0.40
1:A:14:ILE:HG23	1:A:51:VAL:CG2	2.38	0.40
1:E:145:VAL:HG12	1:E:146:ILE:N	2.37	0.40
1:E:18:ASP:OD1	1:E:19:THR:HG22	2.22	0.40
1:E:412:ILE:CG2	1:E:413:ASN:N	2.84	0.40
1:F:263:GLN:N	1:F:263:GLN:NE2	2.69	0.40
1:F:98:ILE:HD13	1:F:98:ILE:C	2.42	0.40
1:A:229:VAL:HG13	1:A:422:VAL:CG2	2.52	0.40
1:A:91:ILE:N	1:A:91:ILE:CD1	2.70	0.40
1:C:288:ARG:O	1:C:289:PHE:HB2	2.22	0.40
1:C:355:ASN:HD22	1:C:400:ASN:HD22	0.82	0.40
1:D:313:PRO:HG3	1:D:332:GLN:HA	2.03	0.40
1:E:20:LYS:HA	1:E:23:GLU:OE1	2.22	0.40
1:E:307:ASP:OD2	1:E:371:SER:HB3	2.21	0.40
1:E:232:ARG:CG	1:E:422:VAL:HG11	2.51	0.40
1:B:49:THR:OG1	1:B:67:ASP:HB3	2.21	0.40
1:F:127:GLY:O	1:F:130:LEU:N	2.55	0.40
1:F:146:ILE:HD12	1:F:164:LEU:HD21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:OG	1:D:56:SER:OG[1_556]	1.98	0.22

## 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	400/431 (93%)	343 (86%)	45 (11%)	12 (3%)	5	12
1	B	398/431 (92%)	337 (85%)	55 (14%)	6 (2%)	13	31
1	C	392/431 (91%)	311 (79%)	56 (14%)	25 (6%)	2	2
1	D	393/431 (91%)	326 (83%)	52 (13%)	15 (4%)	4	8
1	E	377/431 (88%)	315 (84%)	52 (14%)	10 (3%)	6	15
1	F	372/431 (86%)	296 (80%)	59 (16%)	17 (5%)	3	5
All	All	2332/2586 (90%)	1928 (83%)	319 (14%)	85 (4%)	4	9

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ILE
1	A	331	GLU
1	B	178	ASN
1	C	39	SER
1	C	64	ALA
1	C	308	MSE
1	C	313	PRO
1	C	318	PRO
1	C	319	PRO
1	C	382	ASP
1	D	56	SER
1	D	64	ALA
1	D	125	SER
1	D	178	ASN
1	D	276	TYR
1	D	277	VAL
1	D	331	GLU
1	E	89	ALA
1	E	221	VAL
1	E	245	ALA

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Mol	Chain	Res	Type
1	E	313	PRO
1	E	333	VAL
1	F	42	SER
1	F	64	ALA
1	F	114	GLN
1	F	178	ASN
1	F	200	GLU
1	A	42	SER
1	A	174	CYS
1	A	212	PHE
1	A	289	PHE
1	B	245	ALA
1	B	304	GLY
1	B	372	ALA
1	B	403	CYS
1	C	37	SER
1	C	173	ILE
1	C	220	GLY
1	C	275	ASP
1	C	289	PHE
1	C	307	ASP
1	C	316	THR
1	D	78	HIS
1	D	93	GLY
1	D	275	ASP
1	D	320	GLU
1	E	43	SER
1	E	332	GLN
1	F	170	VAL
1	F	286	SER
1	B	289	PHE
1	C	56	SER
1	C	326	ILE
1	C	327	HIS
1	D	289	PHE
1	D	379	ASP
1	F	43	SER
1	F	96	ILE
1	F	190	ALA
1	F	259	GLY
1	A	44	PHE
1	C	8	SER

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Mol	Chain	Res	Type
1	C	178	ASN
1	C	331	GLU
1	C	355	ASN
1	A	64	ALA
1	A	376	PRO
1	A	382	ASP
1	C	94	LEU
1	D	70	PRO
1	E	71	SER
1	E	382	ASP
1	F	221	VAL
1	F	379	ASP
1	F	421	LEU
1	A	170	VAL
1	C	366	PRO
1	D	170	VAL
1	F	150	VAL
1	C	196	ILE
1	E	376	PRO
1	A	318	PRO
1	C	197	GLY
1	F	193	GLY
1	F	376	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/353 (97%)	298 (87%)	45 (13%)	5	11
1	B	341/353 (97%)	295 (86%)	46 (14%)	5	10
1	C	338/353 (96%)	294 (87%)	44 (13%)	5	12
1	D	339/353 (96%)	287 (85%)	52 (15%)	3	8
1	E	324/353 (92%)	283 (87%)	41 (13%)	5	12
1	F	320/353 (91%)	278 (87%)	42 (13%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2005/2118 (95%)	1735 (86%)	270 (14%)	5 10

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	29	GLU
1	A	35	LEU
1	A	44	PHE
1	A	58	LYS
1	A	69	VAL
1	A	72	LYS
1	A	76	SER
1	A	91	ILE
1	A	94	LEU
1	A	105	THR
1	A	113	GLU
1	A	115	ASN
1	A	122	LEU
1	A	131	LEU
1	A	156	GLU
1	A	184	LEU
1	A	199	LEU
1	A	217	THR
1	A	219	PHE
1	A	221	VAL
1	A	226	VAL
1	A	227	ASN
1	A	240	THR
1	A	248	VAL
1	A	265	VAL
1	A	266	LEU
1	A	285	ASP
1	A	286	SER
1	A	288	ARG
1	A	299	LEU
1	A	306	LEU
1	A	315	THR
1	A	321	PHE
1	A	323	GLN
1	A	332	GLN
1	A	334	SER

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Mol	Chain	Res	Type
1	A	337	ARG
1	A	354	LEU
1	A	373	LEU
1	A	390	THR
1	A	393	LEU
1	A	395[A]	MSE
1	A	395[B]	MSE
1	A	416	GLU
1	B	8	SER
1	B	19	THR
1	B	29	GLU
1	B	35	LEU
1	B	39	SER
1	B	54	SER
1	B	60	THR
1	B	69	VAL
1	B	72	LYS
1	B	75	LEU
1	B	76	SER
1	B	94	LEU
1	B	111	ASN
1	B	113	GLU
1	B	115	ASN
1	B	122	LEU
1	B	129	SER
1	B	131	LEU
1	B	140	ILE
1	B	177	ASN
1	B	178	ASN
1	B	182	VAL
1	B	196	ILE
1	B	199	LEU
1	B	219	PHE
1	B	226	VAL
1	B	229	VAL
1	B	233	LEU
1	B	248	VAL
1	B	265	VAL
1	B	271	THR
1	B	278	VAL
1	B	288	ARG
1	B	299	LEU

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Mol	Chain	Res	Type
1	B	306	LEU
1	B	309	VAL
1	B	315	THR
1	B	321	PHE
1	B	323	GLN
1	B	332	GLN
1	B	333	VAL
1	B	337	ARG
1	B	354	LEU
1	B	395	MSE
1	B	421	LEU
1	B	426	LEU
1	C	7	ASN
1	C	10	ARG
1	C	24	LEU
1	C	29	GLU
1	C	42	SER
1	C	44	PHE
1	C	51	VAL
1	C	58	LYS
1	C	60	THR
1	C	71	SER
1	C	72	LYS
1	C	96	ILE
1	C	98	ILE
1	C	122	LEU
1	C	129	SER
1	C	131	LEU
1	C	133	SER
1	C	185	SER
1	C	196	ILE
1	C	199	LEU
1	C	219	PHE
1	C	226	VAL
1	C	229	VAL
1	C	240	THR
1	C	257	VAL
1	C	265	VAL
1	C	288	ARG
1	C	299	LEU
1	C	306	LEU
1	C	316	THR

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Mol	Chain	Res	Type
1	C	328	GLU
1	C	334	SER
1	C	335	LEU
1	C	336	MSE
1	C	354	LEU
1	C	359	SER
1	C	361	VAL
1	C	379	ASP
1	C	384	GLU
1	C	388	CYS
1	C	390	THR
1	C	395	MSE
1	C	403	CYS
1	C	416	GLU
1	D	24	LEU
1	D	33	SER
1	D	35	LEU
1	D	40	ASN
1	D	44	PHE
1	D	45	LYS
1	D	55	THR
1	D	58	LYS
1	D	61	ASN
1	D	72	LYS
1	D	91	ILE
1	D	94	LEU
1	D	99	MSE
1	D	115	ASN
1	D	122	LEU
1	D	131	LEU
1	D	156	GLU
1	D	168	PRO
1	D	178	ASN
1	D	199	LEU
1	D	212	PHE
1	D	213	THR
1	D	219	PHE
1	D	226	VAL
1	D	229	VAL
1	D	231	GLU
1	D	240	THR
1	D	241	LEU

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Mol	Chain	Res	Type
1	D	257	VAL
1	D	265	VAL
1	D	266	LEU
1	D	267	ASP
1	D	275	ASP
1	D	288	ARG
1	D	299	LEU
1	D	301	LEU
1	D	306	LEU
1	D	321	PHE
1	D	324	ARG
1	D	328	GLU
1	D	330	ASN
1	D	332	GLN
1	D	335	LEU
1	D	337	ARG
1	D	354	LEU
1	D	371	SER
1	D	388	CYS
1	D	390	THR
1	D	393	LEU
1	D	399	ASN
1	D	401	GLU
1	D	403	CYS
1	E	10	ARG
1	E	29	GLU
1	E	35	LEU
1	E	51	VAL
1	E	59	GLU
1	E	69	VAL
1	E	72	LYS
1	E	79	THR
1	E	92	ARG
1	E	94	LEU
1	E	99	MSE
1	E	113	GLU
1	E	122	LEU
1	E	125	SER
1	E	131	LEU
1	E	156	GLU
1	E	157	SER
1	E	176	ILE

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Mol	Chain	Res	Type
1	E	182	VAL
1	E	213	THR
1	E	217	THR
1	E	219	PHE
1	E	229	VAL
1	E	257	VAL
1	E	263	GLN
1	E	265	VAL
1	E	271	THR
1	E	277	VAL
1	E	288	ARG
1	E	299	LEU
1	E	306	LEU
1	E	314	LYS
1	E	331	GLU
1	E	335	LEU
1	E	336	MSE
1	E	337	ARG
1	E	354	LEU
1	E	371	SER
1	E	388	CYS
1	E	416	GLU
1	E	424	SER
1	F	25	ARG
1	F	35	LEU
1	F	40	ASN
1	F	41	LYS
1	F	43	SER
1	F	55	THR
1	F	56	SER
1	F	60	THR
1	F	69	VAL
1	F	77	CYS
1	F	94	LEU
1	F	96	ILE
1	F	98	ILE
1	F	99	MSE
1	F	105	THR
1	F	108	SER
1	F	122	LEU
1	F	131	LEU
1	F	156	GLU

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Mol	Chain	Res	Type
1	F	157	SER
1	F	178	ASN
1	F	199	LEU
1	F	213	THR
1	F	219	PHE
1	F	222	THR
1	F	226	VAL
1	F	240	THR
1	F	263	GLN
1	F	265	VAL
1	F	271	THR
1	F	288	ARG
1	F	299	LEU
1	F	310	ASN
1	F	337	ARG
1	F	379	ASP
1	F	388	CYS
1	F	389	LEU
1	F	396	LEU
1	F	402	ARG
1	F	403	CYS
1	F	416	GLU
1	F	426	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	115	ASN
1	A	186	ASN
1	A	227	ASN
1	A	330	ASN
1	A	332	GLN
1	A	343	ASN
1	A	404	GLN
1	B	7	ASN
1	B	61	ASN
1	B	111	ASN
1	B	177	ASN
1	B	186	ASN
1	B	209	ASN
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	399	ASN
1	B	413	ASN
1	C	114	GLN
1	C	178	ASN
1	C	186	ASN
1	C	227	ASN
1	C	327	HIS
1	C	355	ASN
1	C	413	ASN
1	D	111	ASN
1	D	154	GLN
1	D	177	ASN
1	D	178	ASN
1	D	227	ASN
1	D	322	GLN
1	D	355	ASN
1	D	399	ASN
1	D	413	ASN
1	E	7	ASN
1	E	30	HIS
1	E	36	ASN
1	E	227	ASN
1	E	263	GLN
1	E	343	ASN
1	E	413	ASN
1	F	7	ASN
1	F	111	ASN
1	F	177	ASN
1	F	186	ASN
1	F	227	ASN
1	F	343	ASN
1	F	400	ASN
1	F	413	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	TLA	A	501	-	3,9,9	0.43	0	6,12,12	0.81	0
2	TLA	B	501	-	3,9,9	0.74	0	6,12,12	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	A	501	-	-	0/4/12/12	0/0/0/0
2	TLA	B	501	-	-	0/4/12/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TLA	2	0

## 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	397/431 (92%)	-0.12	8 (2%) 68 69	20, 56, 97, 121	0
1	B	395/431 (91%)	0.09	9 (2%) 64 64	24, 65, 111, 128	0
1	C	392/431 (90%)	-0.10	7 (1%) 71 72	28, 58, 107, 140	0
1	D	393/431 (91%)	-0.13	8 (2%) 68 69	27, 55, 98, 125	0
1	E	378/431 (87%)	0.28	32 (8%) 13 11	25, 74, 115, 135	0
1	F	372/431 (86%)	0.18	16 (4%) 39 39	30, 78, 115, 166	0
All	All	2327/2586 (89%)	0.03	80 (3%) 49 49	20, 63, 109, 166	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	335	LEU	7.0
1	E	279	GLY	6.1
1	C	40	ASN	5.4
1	B	326	ILE	5.3
1	E	79	THR	4.5
1	A	318	PRO	4.4
1	E	278	VAL	4.3
1	E	403	CYS	4.1
1	E	114	GLN	4.0
1	E	281	VAL	3.8
1	E	88	PHE	3.8
1	C	316	THR	3.8
1	E	44	PHE	3.8
1	C	315	THR	3.7
1	A	321	PHE	3.7
1	A	322	GLN	3.7
1	E	407	VAL	3.6
1	A	326	ILE	3.6
1	F	276	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	334	SER	3.5
1	E	428	ILE	3.4
1	E	361	VAL	3.4
1	E	274	ALA	3.4
1	C	345	LYS	3.3
1	E	423	ASP	3.3
1	B	322	GLN	3.3
1	E	354	LEU	3.3
1	E	43	SER	3.2
1	A	335	LEU	3.2
1	D	315	THR	3.2
1	A	315	THR	3.2
1	D	57	TRP	3.1
1	F	309	VAL	3.1
1	E	280	GLY	3.1
1	E	427	GLU	3.1
1	E	430	PRO	3.0
1	B	328	GLU	3.0
1	F	426	LEU	3.0
1	F	297	ILE	3.0
1	B	332	GLN	2.8
1	E	277	VAL	2.8
1	E	309	VAL	2.8
1	D	323	GLN	2.8
1	E	375	ALA	2.8
1	B	378	LYS	2.7
1	F	333	VAL	2.7
1	E	293	LEU	2.7
1	A	79	THR	2.7
1	E	311	PHE	2.6
1	F	97	ALA	2.6
1	F	362	CYS	2.6
1	E	232	ARG	2.6
1	B	318	PRO	2.6
1	F	393	LEU	2.5
1	C	41	LYS	2.4
1	E	266	LEU	2.4
1	F	399	ASN	2.4
1	D	326	ILE	2.4
1	C	314	LYS	2.4
1	B	314	LYS	2.3
1	D	319	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	367	GLU	2.3
1	D	321	PHE	2.3
1	B	319	PRO	2.3
1	F	403	CYS	2.3
1	E	237	GLY	2.3
1	E	110	ALA	2.3
1	D	320	GLU	2.3
1	E	292	ILE	2.3
1	F	273	VAL	2.3
1	F	311	PHE	2.2
1	F	359	SER	2.2
1	B	368	LYS	2.1
1	F	335	LEU	2.1
1	C	44	PHE	2.1
1	E	78	HIS	2.1
1	F	212	PHE	2.1
1	A	319	PRO	2.0
1	F	75	LEU	2.0
1	D	322	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	TLA	A	501	10/10	0.92	0.16	0.59	72,74,80,86	0
2	TLA	B	501	10/10	0.86	0.18	0.14	75,85,90,91	0

## 6.5 Other polymers

There are no such residues in this entry.