



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:18 PM UTC

PDB ID : 3WRW / pdb_00003wrw
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

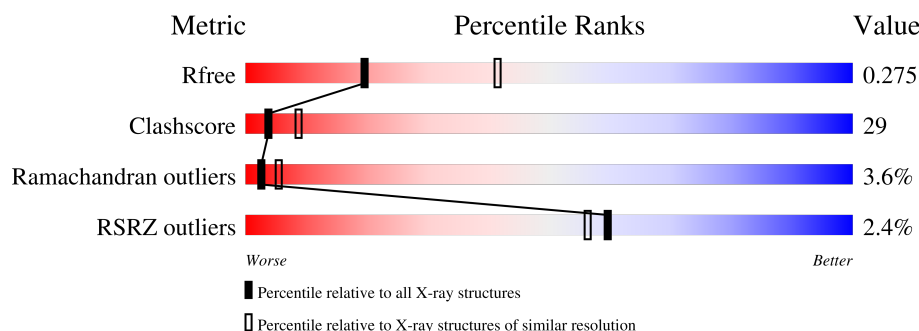
1 Overall quality at a glance

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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
RSRZ outliers	180081	4348 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	% 54% 38% • 6%
1	B	431	% 53% 38% • 6%
1	C	431	2% 47% 41% 5% 7%
1	D	431	% 52% 37% • 7%
1	E	431	4% 54% 32% • 10%
1	F	431	3% 47% 38% • 12%

2 Entry composition [i](#)

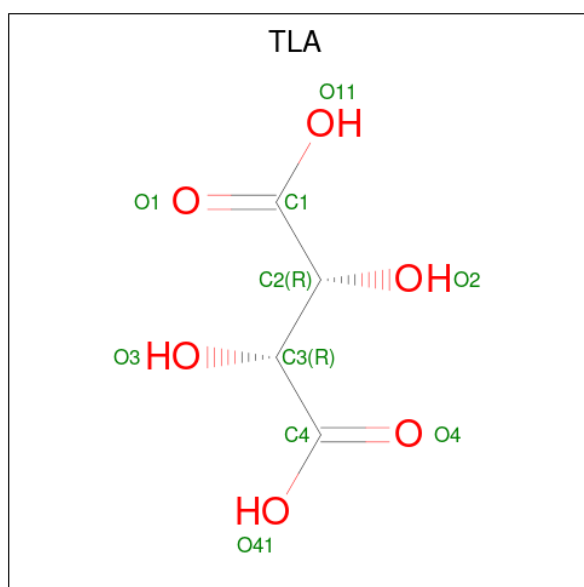
There are 3 unique types of molecules in this entry. The entry contains 17863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: TLA) (formula: C₄H₆O₆).



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		

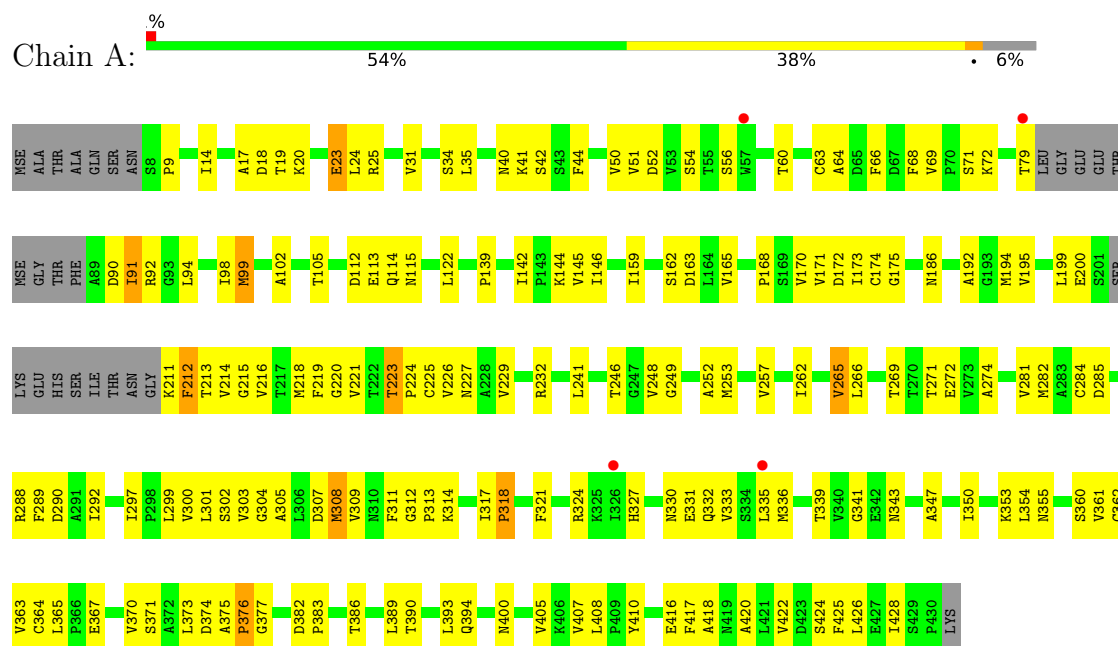
- Molecule 3 is water.

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		

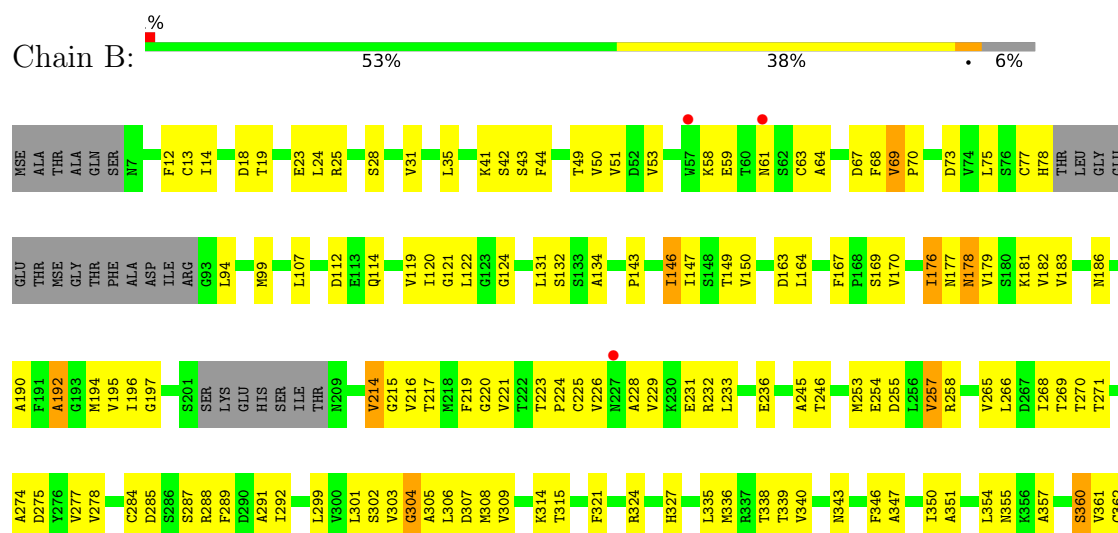
3 Residue-property plots

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

• Molecule 1: Tm-1 protein

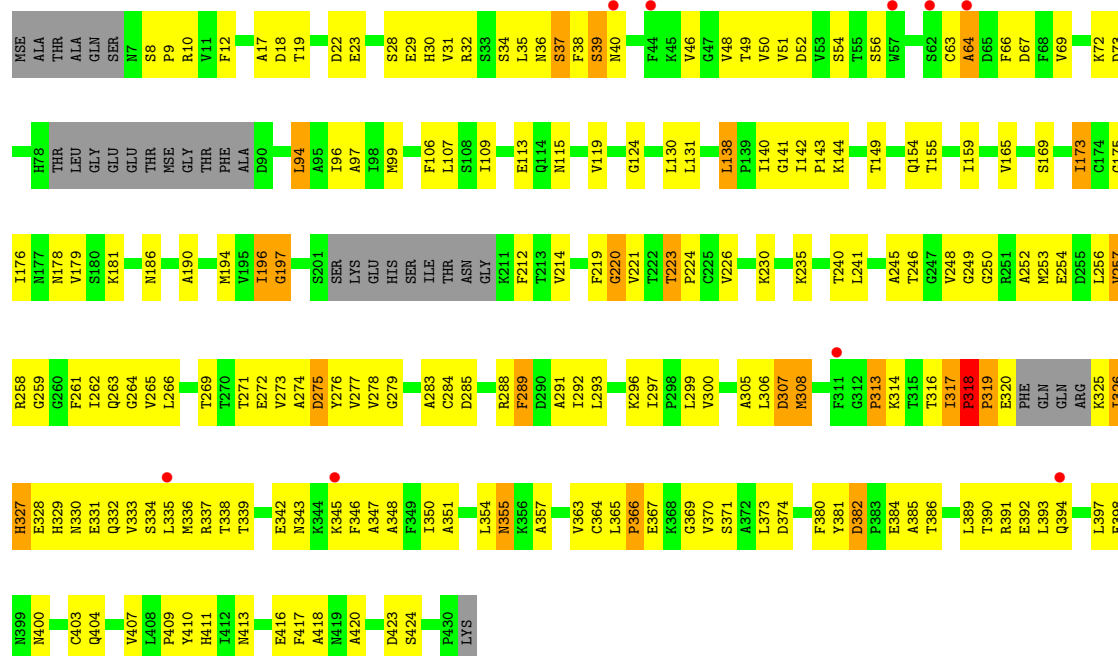


• Molecule 1: Tm-1 protein

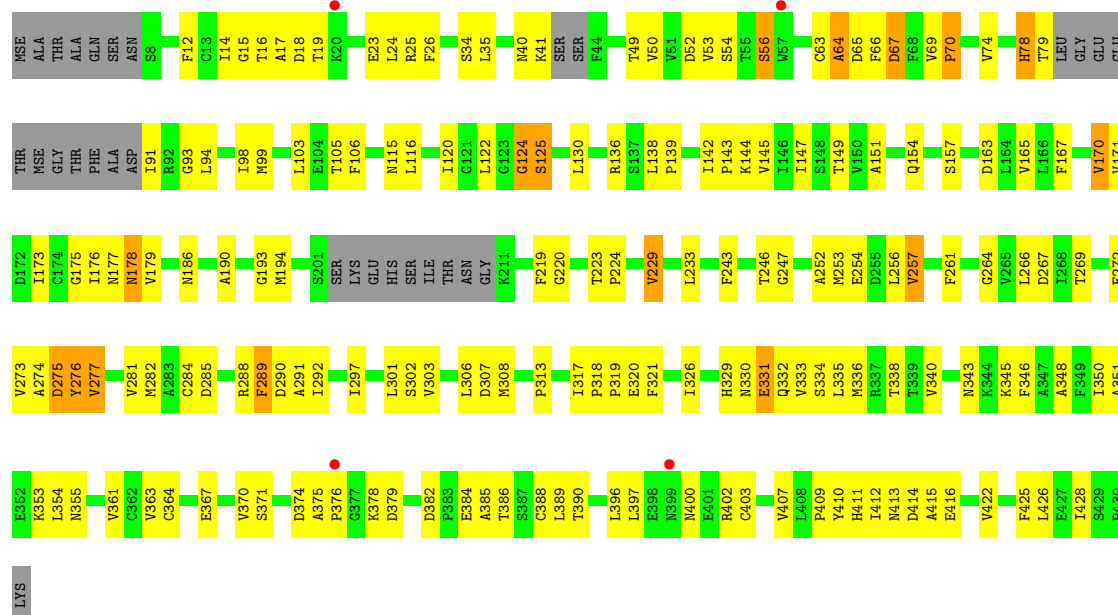




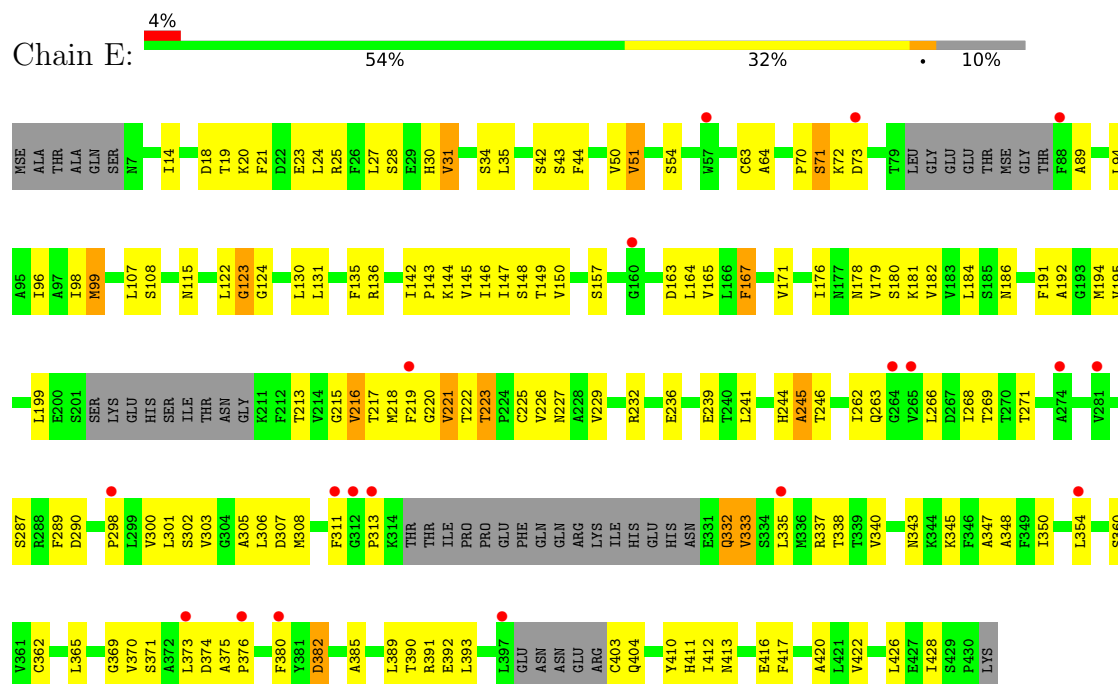
• Molecule 1: Tm-1 protein



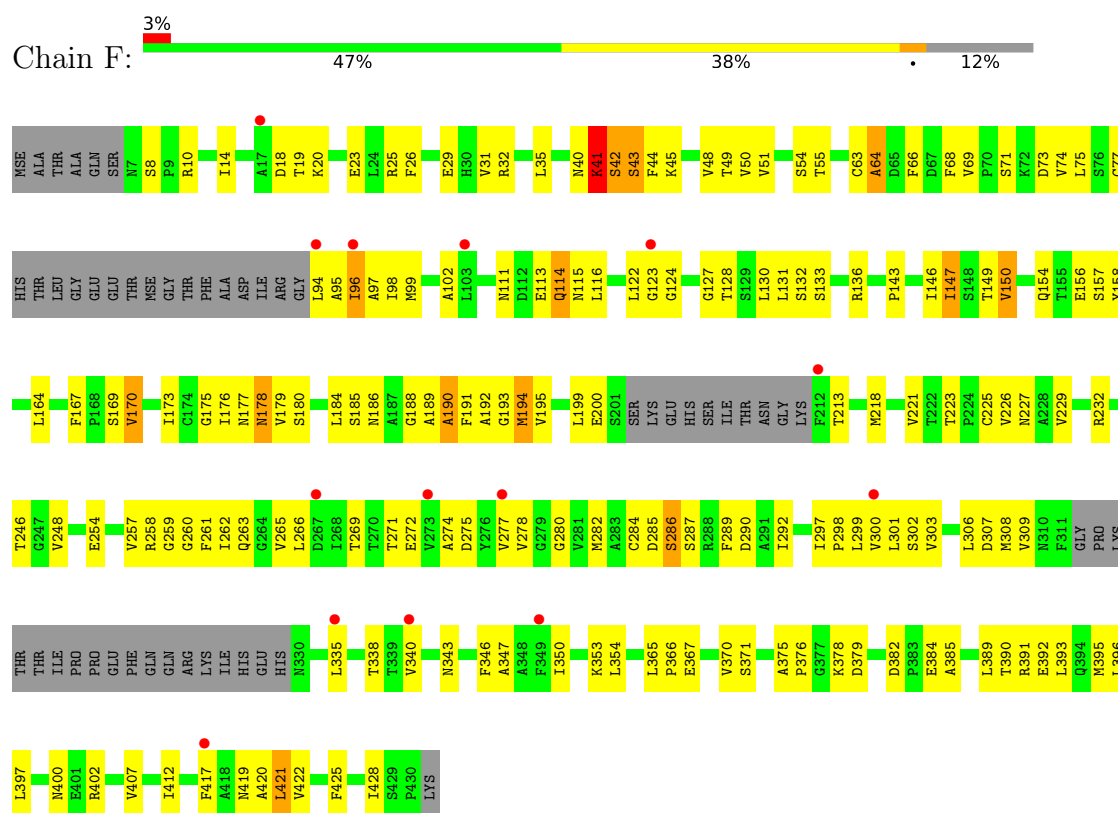
• Molecule 1: Tm-1 protein



• 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, α , β , γ	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) 95.0 (49.64-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.278 (Not available) , 0.275	Depositor DCC
R_{free} test set	3975 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.95	1/3088 (0.0%)	1.08	9/4167 (0.2%)
1	B	0.91	2/3070 (0.1%)	1.07	7/4143 (0.2%)
1	C	0.95	1/3034 (0.0%)	1.10	10/4094 (0.2%)
1	D	0.98	0/3054	1.15	8/4120 (0.2%)
1	E	0.93	0/2918	1.09	10/3934 (0.3%)
1	F	0.82	1/2867 (0.0%)	1.04	5/3868 (0.1%)
All	All	0.92	5/18031 (0.0%)	1.09	49/24326 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	E	0	1
1	F	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	318	PRO	CA-C	6.26	1.57	1.52
1	A	200	GLU	CA-C	5.54	1.59	1.53
1	F	395	MSE	SE-CE	-5.16	1.79	1.95
1	B	192	ALA	CA-C	5.09	1.59	1.52
1	B	176	ILE	N-CA	-5.03	1.40	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	MSE	N-CA-C	-7.78	102.75	111.07
1	C	223	THR	CA-C-N	-7.48	110.49	119.84
1	C	223	THR	C-N-CA	-7.48	110.49	119.84
1	E	99	MSE	N-CA-C	-7.12	102.57	111.11
1	C	317	ILE	CA-C-N	7.07	127.66	120.38
1	C	317	ILE	C-N-CA	7.07	127.66	120.38
1	E	223	THR	CA-C-N	-7.02	111.67	118.97
1	E	223	THR	C-N-CA	-7.02	111.67	118.97
1	D	229	VAL	N-CA-CB	6.92	119.95	110.54
1	D	171	VAL	N-CA-C	-6.91	100.10	108.53
1	C	318	PRO	N-CA-C	6.88	119.10	110.70
1	B	257	VAL	N-CA-CB	6.82	118.53	110.55
1	A	223	THR	CA-C-N	-6.78	112.19	119.24
1	A	223	THR	C-N-CA	-6.78	112.19	119.24
1	C	257	VAL	N-CA-C	-6.26	104.41	110.42
1	C	257	VAL	N-CA-CB	6.23	117.84	110.55
1	F	194	MSE	N-CA-C	-6.22	104.41	111.07
1	D	257	VAL	N-CA-CB	6.21	119.46	110.52
1	E	311	PHE	N-CA-C	6.15	116.68	108.38
1	D	124	GLY	N-CA-C	-6.14	104.34	112.81
1	D	67	ASP	N-CA-C	-6.03	102.41	110.24
1	B	214	VAL	N-CA-C	-5.95	100.85	109.29
1	D	138	LEU	CA-C-N	5.93	125.87	119.76
1	D	138	LEU	C-N-CA	5.93	125.87	119.76
1	E	31	VAL	N-CA-C	-5.93	105.94	111.45
1	E	167	PHE	CA-C-N	5.84	126.76	119.98
1	E	167	PHE	C-N-CA	5.84	126.76	119.98
1	E	142	ILE	CB-CA-C	-5.83	103.97	110.68
1	B	360	SER	N-CA-C	5.64	117.58	110.24
1	F	147	ILE	N-CA-C	-5.58	101.85	109.55
1	B	69	VAL	CA-C-N	5.56	125.54	120.03
1	B	69	VAL	C-N-CA	5.56	125.54	120.03
1	B	146	ILE	CB-CA-C	-5.47	102.68	110.12
1	C	138	LEU	CA-C-N	5.46	126.66	119.84
1	C	138	LEU	C-N-CA	5.46	126.66	119.84
1	E	51	VAL	N-CA-C	5.45	115.70	107.75
1	F	45	LYS	N-CA-C	-5.42	101.71	110.32
1	A	195	VAL	N-CA-C	5.38	115.59	110.53
1	E	216	VAL	N-CA-C	5.38	115.64	108.27
1	B	190	ALA	N-CA-C	-5.34	105.15	110.97
1	D	413	ASN	N-CA-C	5.31	119.74	113.16
1	A	341	GLY	N-CA-C	-5.21	106.11	112.77
1	F	29	GLU	N-CA-C	-5.19	105.31	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	MSE	N-CA-C	5.16	116.91	109.07
1	C	124	GLY	N-CA-C	-5.15	104.69	112.41
1	F	41	LYS	N-CA-C	5.12	116.98	107.60
1	A	23	GLU	N-CA-C	-5.08	105.82	111.36
1	A	265	VAL	N-CA-C	5.05	115.55	108.17
1	A	333	VAL	N-CA-C	5.02	115.20	107.77

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	156	1
1	B	3027	0	3039	166	0
1	C	2996	0	3013	202	0
1	D	3015	0	3038	175	1
1	E	2881	0	2907	166	0
1	F	2835	0	2850	193	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	1030	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 29.

All (1030) 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
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:HD12	1:E:147:ILE:N	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:94:LEU:HD23	1:E:98:ILE:HD11	1.55	0.88
1:E:225:CYS:O	1:E:229:VAL:HG12	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:90:ASP:C	1:A:91:ILE:HD13	2.09	0.77
1:E:147:ILE:HD12	1:E:147:ILE:H	1.47	0.77
1:A:91:ILE:HD13	1:A:91:ILE:N	1.98	0.77
1:B:269:THR:HG22	1:B:271:THR:HG22	1.67	0.77
1:C:130:LEU:HD23	1:C:130:LEU:C	2.10	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:265:VAL:HG22	1:F:299:LEU:HD23	1.67	0.76
1:F:269:THR:HG22	1:F:271:THR:HG22	1.67	0.76
1:C:313:PRO:C	1:C:317:ILE:HG21	2.10	0.76
1:D:350:ILE:HG22	1:D:354:LEU:HD22	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:F:49:THR:O	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LEU:HD22	1:C:131:LEU:HD13	1.72	0.71
1:F:173:ILE:O	1:F:173:ILE:HG22	1.89	0.71
1:C:274:ALA:O	1:C:275:ASP:C	2.34	0.70
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
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:41:LYS:N	1:F:42:SER:HB2	2.08	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: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:D:124:GLY:O	1:D:125:SER:C	2.37	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:D:63:CYS:O	1:D:64:ALA:C	2.38	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:63:CYS:O	1:F:64:ALA:C	2.38	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:E:266:LEU:HD13	1:E:300:VAL:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HG12	1:A:426:LEU:HD23	1.77	0.65
1:C:18:ASP:OD1	1:C:19:THR:N	2.30	0.65
1:C:179:VAL:HG21	1:D:256:LEU:HD13	1.78	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:OE1	1:C:320:GLU:N	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
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: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:74:VAL:CG1	1:D:99:MSE:SE	2.96	0.63
1:D:290:ASP:OD1	1:D:353:LYS:NZ	2.31	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:246:THR:HG22	1:F:246:THR:O	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:211:LYS:O	1:A:212:PHE:C	2.41	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:A:371:SER:HG	1:A:373:LEU:H	1.47	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:C:354:LEU:O	1:C:357:ALA:HB2	1.99	0.62
1:E:94:LEU:CD2	1:E:98:ILE:HD11	2.28	0.62
1:E:360:SER:CB	1:E:428:ILE:HG23	2.28	0.62
1:F:35:LEU:HD11	1:F:195:VAL:CG2	2.29	0.62
1:B:122:LEU:HD12	1:B:122:LEU:C	2.25	0.62
1:D:144:LYS:O	1:D:165:VAL:HG12	1.98	0.62
1:E:219:PHE:O	1:E:220:GLY:C	2.43	0.62
1:F:40:ASN:C	1:F:42:SER:HB2	2.25	0.62
1:D:264:GLY:HA2	1:D:297:ILE:HD12	1.82	0.62
1:D:301:LEU:HD23	1:D:301:LEU:C	2.24	0.62
1:B:122:LEU:C	1:B:122:LEU:CD1	2.73	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:HE21	1:A:332:GLN:HA	1.65	0.61
1:C:328:GLU:OE1	1:C:330:ASN:N	2.34	0.61
1:E:71:SER:O	1:E:72:LYS:C	2.41	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:E:34:SER:O	1:E:35:LEU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:HD23	1:B:302:SER:N	2.16	0.60
1:C:335:LEU:HD23	1:C:335:LEU:N	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:N	1:D:335:LEU:CD2	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:B:24:LEU:HD23	1:B:24:LEU:C	2.28	0.59
1:C:275:ASP:O	1:C:279:GLY:N	2.36	0.59
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:E:18:ASP:CG	1:E:54:SER:OG	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:ASN:C	1:F:40:ASN:OD1	2.46	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:E:332:GLN:O	1:E:333:VAL:C	2.46	0.58
1:F:195:VAL:O	1:F:199:LEU:HD22	2.03	0.58
1:C:28:SER:O	1:C:29:GLU:C	2.47	0.58
1:D:375:ALA:HB3	1:D:378:LYS:HG3	1.86	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:C:285:ASP:C	1:C:285:ASP:OD1	2.46	0.57
1:D:139:PRO:HD2	1:D:142:ILE:HD12	1.86	0.57
1:D:193:GLY:O	1:D:194:MSE:C	2.46	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: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
1:B:321:PHE:HB2	1:B:324:ARG:HG3	1.86	0.57
1:D:53:VAL:C	1:D:99:MSE:HE3	2.29	0.57
1:E:298:PRO:HB3	1:E:428:ILE:HG22	1.86	0.57
1:D:334:SER:C	1:D:335:LEU:HD23	2.30	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: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:B:302:SER:OG	1:B:303:VAL:N	2.37	0.56
1:C:106:PHE:C	1:C:106:PHE:CD1	2.82	0.56
1:D:177:ASN:O	1:D:178:ASN:C	2.47	0.56
1:F:55:THR:HG21	1:F:95:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:ILE:O	1:F:354:LEU:HD13	2.05	0.56
1:C:179:VAL:HG22	1:D:261:PHE:CD2	2.41	0.56
1:C:240:THR:O	1:C:240:THR:CG2	2.53	0.56
1:C:264:GLY:HA2	1:C:297:ILE:HD12	1.87	0.56
1:C:273:VAL:CG1	1:C:273:VAL:O	2.53	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: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:O	1:C:246:THR:CG2	2.54	0.56
1:C:355:ASN:HA	1:C:400:ASN:HD21	1.67	0.56
1:D:34:SER:O	1:D:35:LEU:C	2.48	0.56
1:E:289:PHE:CE1	1:E:301:LEU:HD11	2.41	0.56
1:D:91:ILE:N	1:D:91:ILE:CD1	2.67	0.56
1:D:302:SER:OG	1:D:303:VAL:N	2.39	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:32:ARG:HB2	1:C:48:VAL:HG21	1.88	0.56
1:C:38:PHE:O	1:C:40:ASN:N	2.39	0.56
1:C:327:HIS:O	1:C:328:GLU:C	2.49	0.56
1:A:218:MSE:HB2	1:A:226:VAL:HG11	1.88	0.55
1:D:382:ASP:C	1:D:382:ASP:OD1	2.49	0.55
1:F:299:LEU:C	1:F:299:LEU:HD22	2.31	0.55
1:A:360:SER:HB2	1:A:428:ILE:HG23	1.88	0.55
1:B:150:VAL:HG23	1:B:150:VAL:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:HIS:O	1:C:327:HIS:CD2	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:A:34:SER:O	1:A:35:LEU:C	2.48	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:F:96:ILE:HG22	1:F:97:ALA:N	2.21	0.54
1:B:169:SER:C	1:B:170:VAL:HG23	2.32	0.54
1:D:25:ARG:HG3	1:D:63:CYS:SG	2.47	0.54
1:C:334:SER:C	1:C:335:LEU:HD23	2.32	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:O	1:C:273:VAL:HG12	2.08	0.54
1:C:337:ARG:CG	1:C:380:PHE:HB3	2.37	0.54
1:C:347:ALA:CB	1:C:393:LEU:HD22	2.38	0.54
1:D:49:THR:HG22	1:D:50:VAL:N	2.22	0.54
1:D:122:LEU:CD1	1:D:122:LEU:C	2.80	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
1:B:299:LEU:C	1:B:299:LEU:HD22	2.32	0.54
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:O	1:A:94:LEU:HD22	2.08	0.54
1:C:278:VAL:HG12	1:C:278:VAL:O	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:C:130:LEU:C	1:C:130:LEU:CD2	2.81	0.53
1:C:275:ASP:HB3	1:C:283:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:336:MSE:O	1:C:337:ARG:C	2.51	0.53
1:C:410:TYR:CE1	1:C:416:GLU:HG3	2.43	0.53
1:C:96:ILE:HG22	1:C:97:ALA:N	2.22	0.53
1:C:274:ALA:O	1:C:276:TYR:N	2.41	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:D:17:ALA:CB	1:D:52:ASP:CG	2.82	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:F:420:ALA:O	1:F:421:LEU:C	2.52	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:25:ARG:HD2	1:B:64:ALA:HB2	1.91	0.53
1:B:258:ARG:NH2	1:B:291:ALA:HB2	2.23	0.53
1:C:17:ALA:HB3	1:C:52:ASP:OD2	2.08	0.53
1:C:329:HIS:O	1:C:330:ASN:CG	2.52	0.53
1:C:337:ARG:HD2	1:C:338:THR:O	2.08	0.53
1:E:35:LEU:HD13	1:E:192:ALA:HB1	1.91	0.53
1:B:131:LEU:O	1:B:132:SER:C	2.52	0.53
1:B:18:ASP:CG	1:B:19:THR:HG22	2.31	0.53
1:C:299:LEU:C	1:C:299:LEU:CD2	2.81	0.53
1:C:37:SER:O	1:C:40:ASN:HB2	2.08	0.53
1:C:69:VAL:O	1:C:69:VAL:HG22	2.08	0.53
1:E:350:ILE:HG22	1:E:354:LEU:CD2	2.36	0.53
1:B:246:THR:HG22	1:B:246:THR:O	2.07	0.53
1:C:154:GLN:HB2	1:D:154:GLN:HE22	1.74	0.53
1:C:249:GLY:O	1:C:250:GLY:C	2.52	0.53
1:F:14:ILE:HG23	1:F:51:VAL:HG22	1.91	0.53
1:A:285:ASP:OD1	1:A:285:ASP:C	2.52	0.52
1:A:417:PHE:O	1:A:420:ALA:HB3	2.09	0.52
1:D:63:CYS:O	1:D:65:ASP:N	2.42	0.52
1:C:223:THR:O	1:C:224:PRO:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:196:ILE:O	1:C:197:GLY:C	2.53	0.52
1:F:186:ASN:N	1:F:186:ASN:HD22	2.07	0.52
1:A:20:LYS:HG2	1:A:173:ILE:HG22	1.92	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:D:246:THR:O	1:D:246:THR:HG22	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:B:303:VAL:O	1:B:304:GLY:C	2.53	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:C:34:SER:O	1:C:35:LEU:C	2.53	0.51
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: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:F:258:ARG:C	1:F:260:GLY:H	2.18	0.51
1:F:301:LEU:HD23	1:F:301:LEU:C	2.36	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:51:VAL:HG23	1:C:52:ASP:N	2.25	0.51
1:C:214:VAL:CG1	1:C:266:LEU:HD23	2.41	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LEU:HD23	1:C:130:LEU:O	2.10	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: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:D:26:PHE:CD1	1:D:26:PHE:C	2.89	0.51
1:F:122:LEU:HD12	1:F:122:LEU:N	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: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:O	1:A:221:VAL:HG23	2.11	0.50
1:C:343:ASN:HD22	1:C:389:LEU:HD22	1.74	0.50
1:D:17:ALA:HB2	1:D:52:ASP:CG	2.36	0.50
1:C:194:MSE:CG	1:D:190:ALA:HB2	2.41	0.50
1:C:391:ARG:O	1:C:392:GLU:C	2.55	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:F:419:ASN:O	1:F:420:ALA:C	2.53	0.50
1:B:59:GLU:HG2	1:B:61:ASN:HD21	1.76	0.50
1:B:216:VAL:HG13	1:B:268:ILE:CD1	2.40	0.50
1:C:369:GLY:HA3	1:C:374:ASP:O	2.11	0.50
1:D:400:ASN:OD1	1:D:402:ARG:HB2	2.11	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
1:C:155:THR:HG21	1:D:151:ALA:O	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:O	1:B:304:GLY:HA3	2.11	0.49
1:C:10:ARG:NH1	1:C:49:THR:OG1	2.40	0.49
1:C:155:THR:HG23	1:C:159:ILE:HD12	1.93	0.49
1:C:319:PRO:O	1:C:320:GLU:C	2.55	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:D:94:LEU:O	1:D:94:LEU:HD22	2.11	0.49
1:D:274:ALA:O	1:D:276:TYR:N	2.45	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:24:LEU:CD1	1:D:50:VAL:HG13	2.36	0.49
1:D:253:MSE:O	1:D:257:VAL:HG13	2.12	0.49
1:E:96:ILE:HG23	1:E:130:LEU:HB2	1.94	0.49
1:E:410:TYR:CE1	1:E:416:GLU:HG3	2.48	0.49
1:A:229:VAL:HG13	1:A:422:VAL:HG22	1.93	0.49
1:A:360:SER:O	1:A:361:VAL:HG23	2.12	0.49
1:C:94:LEU:HD13	1:C:94:LEU:C	2.38	0.49
1:E:25:ARG:HG3	1:E:63:CYS:SG	2.53	0.49
1:E:195:VAL:O	1:E:199:LEU:HD13	2.13	0.49
1:F:391:ARG:O	1:F:392:GLU:C	2.55	0.49
1:A:71:SER:O	1:A:72:LYS:C	2.52	0.49
1:C:235:LYS:HB2	1:C:235:LYS:NZ	2.28	0.49
1:D:18:ASP:CG	1:D:54:SER:HG	2.19	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:232:ARG:CG	1:B:422:VAL:HG11	2.43	0.49
1:D:177:ASN:ND2	1:D:179:VAL:H	2.10	0.49
1:F:74:VAL:CG2	1:F:99:MSE:CE	2.88	0.49
1:F:275:ASP:HA	1:F:309:VAL:CG1	2.42	0.49
1:F:275:ASP:CG	1:F:309:VAL:HG13	2.37	0.49
1:C:245:ALA:HB1	1:C:272:GLU:HG3	1.95	0.48
1:F:99:MSE:O	1:F:102:ALA:CB	2.61	0.48
1:F:347:ALA:HA	1:F:393:LEU:HD21	1.94	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: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:E:31:VAL:HG12	1:E:35:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ALA:CB	1:F:309:VAL:HG22	2.42	0.48
1:D:274:ALA:O	1:D:275:ASP:C	2.56	0.48
1:D:330:ASN:O	1:D:331:GLU:C	2.56	0.48
1:E:410:TYR:CD1	1:E:416:GLU:HG3	2.48	0.48
1:F:69:VAL:HG23	1:F:73:ASP:HB2	1.94	0.48
1:F:412:ILE:HA	1:F:417:PHE:CD2	2.48	0.48
1:A:122:LEU:HD12	1:A:122:LEU:H	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:D:284:CYS:HB2	1:D:288:ARG:HG2	1.94	0.48
1:E:27:LEU:O	1:E:28:SER:C	2.56	0.48
1:B:419:ASN:O	1:B:423:ASP:CG	2.57	0.48
1:C:119:VAL:HG23	1:C:119:VAL:O	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:D:144:LYS:NZ	1:D:163:ASP:OD1	2.37	0.48
1:E:303:VAL:CA	1:E:306:LEU:HD22	2.44	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: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:B:69:VAL:HG22	1:B:69:VAL:O	2.12	0.48
1:B:225:CYS:O	1:B:229:VAL:HG13	2.12	0.48
1:B:351:ALA:HA	1:B:397:LEU:HD21	1.94	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:F:51:VAL:HA	1:F:69:VAL:HG13	1.95	0.48
1:F:169:SER:O	1:F:170:VAL:HB	2.13	0.48
1:B:265:VAL:HG11	1:B:292:ILE:CD1	2.44	0.47
1:C:69:VAL:O	1:C:69:VAL:CG2	2.62	0.47
1:D:281:VAL:HG12	1:D:281:VAL:O	2.14	0.47
1:E:220:GLY:O	1:E:222:THR:N	2.47	0.47
1:F:258:ARG:C	1:F:260:GLY:N	2.71	0.47
1:A:281:VAL:HG13	1:A:282:MSE:HG3	1.96	0.47
1:C:417:PHE:O	1:C:418:ALA:C	2.57	0.47
1:D:17:ALA:CB	1:D:52:ASP:OD2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:PHE:O	1:D:290:ASP:C	2.57	0.47
1:E:122:LEU:HD12	1:E:122:LEU:H	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:384:GLU:HG2	1:C:385:ALA:N	2.29	0.47
1:D:428:ILE:O	1:D:428:ILE:CG2	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:B:219:PHE:O	1:B:220:GLY:C	2.58	0.47
1:C:109:ILE:CG2	1:C:109:ILE:O	2.62	0.47
1:C:109:ILE:O	1:C:109:ILE:HG22	2.15	0.47
1:C:190:ALA:HB2	1:D:194:MSE:HG2	1.96	0.47
1:D:176:ILE:HD13	1:D:176:ILE:N	2.29	0.47
1:A:90:ASP:CA	1:A:91:ILE:HD13	2.44	0.47
1:B:214:VAL:HG12	1:B:215:GLY:N	2.30	0.47
1:C:257:VAL:HG12	1:C:262:ILE:CG2	2.45	0.47
1:E:239:GLU:OE2	1:F:177:ASN:HB2	2.15	0.47
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:32:ARG:NH1	1:F:66:PHE:CE1	2.83	0.47
1:F:343:ASN:HD21	1:F:385:ALA:HB1	1.79	0.47
1:A:35:LEU:HD12	1:A:35:LEU:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:O	1:E:108:SER:C	2.58	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: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:19:THR:O	1:C:19:THR:HG22	2.14	0.46
1:C:22:ASP:O	1:C:176:ILE:HD11	2.15	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:264:GLY:CA	1:D:297:ILE:HD12	2.44	0.46
1:E:31:VAL:O	1:E:35:LEU:HD22	2.15	0.46
1:E:123:GLY:O	1:E:148:SER:HA	2.16	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
1:C:63:CYS:O	1:C:64:ALA:C	2.58	0.46
1:C:165:VAL:HG21	1:D:167:PHE:CE2	2.50	0.46
1:D:94:LEU:HD22	1:D:98:ILE:HG13	1.96	0.46
1:D:219:PHE:HB2	1:D:269:THR:HG21	1.97	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:335:LEU:N	1:C:335:LEU:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:CYS:O	1:B:392:GLU:HB2	2.16	0.45
1:C:9:PRO:HG2	1:C:46:VAL:HG22	1.98	0.45
1:C:308:MSE:SE	1:C:335:LEU:CD1	3.14	0.45
1:E:94:LEU:HD23	1:E:98:ILE:CD1	2.38	0.45
1:A:25:ARG:HG3	1:A:63:CYS:SG	2.56	0.45
1:D:306:LEU:HA	1:D:306:LEU:HD12	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:98:ILE:C	1:F:98:ILE:HD13	2.42	0.45
1:C:277:VAL:CG2	1:C:278:VAL:N	2.78	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:OD1	1:C:115:ASN:N	2.50	0.45
1:C:140:ILE:HG22	1:C:141:GLY:N	2.32	0.45
1:C:337:ARG:CD	1:C:338:THR:O	2.65	0.45
1:E:165:VAL:HG21	1:F:167:PHE:CE2	2.52	0.45
1:E:373:LEU:HB3	1:E:380:PHE:HB2	1.99	0.45
1:B:77:CYS:O	1:B:78:HIS:C	2.60	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:371:SER:O	1:B:372:ALA:C	2.60	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:C:364:CYS:C	1:C:365:LEU:HD22	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:112:ASP:C	1:B:114:GLN:N	2.75	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:105:THR:O	1:D:106:PHE:C	2.58	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
1:A:375:ALA:O	1:A:376:PRO:C	2.60	0.44
2:A:501:TLA:O1	2:A:501:TLA:O3	2.34	0.44
1:C:72:LYS:O	1:C:73:ASP:C	2.59	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:E:115:ASN:OD1	1:E:115:ASN:N	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:A:60:THR:HG22	1:A:68:PHE:CZ	2.52	0.44
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.79	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: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
1:E:42:SER:C	1:E:44:PHE:H	2.25	0.44
1:F:41:LYS:CA	1:F:42:SER:CB	2.95	0.44
1:F:347:ALA:HB3	1:F:392:GLU:HG3	2.00	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:HD13	1:B:426:LEU:HA	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:223:THR:O	1:B:224:PRO:C	2.57	0.44
1:B:303:VAL:HA	1:B:306:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:PHE:O	1:C:67:ASP:C	2.61	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: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:98:ILE:HD13	1:F:98:ILE:O	2.18	0.44
1:F:292:ILE:HG23	1:F:297:ILE:HD11	1.99	0.44
1:A:90:ASP:OD1	1:A:90:ASP:N	2.50	0.44
1:A:265:VAL:HG11	1:A:292:ILE:HD13	1.99	0.44
1:C:149:THR:HG23	1:C:173:ILE:HD12	2.00	0.44
1:E:42:SER:O	1:E:44:PHE:N	2.51	0.44
1:E:287:SER:CA	1:E:290:ASP:OD2	2.66	0.44
1:D:16:THR:HG22	1:D:54:SER:HA	1.99	0.43
1:D:40:ASN:HA	1:D:41:LYS:HA	1.78	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:D:375:ALA:O	1:D:376:PRO:C	2.61	0.43
1:E:24:LEU:O	1:E:24:LEU:HD13	2.18	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:75:LEU:HD23	1:B:75:LEU:HA	1.85	0.43
1:D:122:LEU:C	1:D:122:LEU:HD12	2.43	0.43
1:D:149:THR:HG23	1:D:173:ILE:HD12	2.00	0.43
1:D:345:LYS:O	1:D:346:PHE:C	2.61	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
1:F:285:ASP:O	1:F:287:SER:N	2.50	0.43
1:A:17:ALA:N	1:A:52:ASP:OD1	2.44	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: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:24:LEU:CD1	1:E:50:VAL:CG1	2.96	0.43
1:E:221:VAL:HG11	1:E:308:MSE:HE1	2.01	0.43
1:F:50:VAL:O	1:F:69:VAL:HG12	2.19	0.43
1:F:226:VAL:HG22	1:F:227:ASN:N	2.33	0.43
1:F:299:LEU:HD22	1:F:300:VAL:N	2.34	0.43
1:D:329:HIS:HB3	1:D:333:VAL:CG2	2.41	0.43
1:A:24:LEU:HD13	1:A:50:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:OD1	1:A:163:ASP:N	2.50	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:B:177:ASN:O	1:B:178:ASN:C	2.61	0.43
1:C:345:LYS:O	1:C:348:ALA:HB3	2.18	0.43
1:C:382:ASP:O	1:C:382:ASP:CG	2.61	0.43
1:C:384:GLU:O	1:C:385:ALA:C	2.60	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: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:189:ALA:O	1:F:190:ALA:C	2.62	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
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:299:LEU:C	1:A:299:LEU:CD2	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:VAL:CB	1:F:99:MSE:HE1	2.49	0.42
1:F:150:VAL:HG21	1:F:158:TYR:OH	2.18	0.42
1:B:314:LYS:HG3	1:B:315:THR:N	2.34	0.42
1:C:212:PHE:CD1	1:C:212:PHE:C	2.97	0.42
1:D:120:ILE:HD11	1:D:147:ILE:HD11	2.02	0.42
1:D:14:ILE:CG2	1:D:15:GLY:N	2.82	0.42
1:D:147:ILE:HD12	1:D:147:ILE:N	2.34	0.42
1:D:220:GLY:C	1:D:223:THR:HG23	2.45	0.42
1:F:177:ASN:O	1:F:178:ASN:C	2.62	0.42
1:F:298:PRO:HB3	1:F:428:ILE:CG2	2.46	0.42
1:A:232:ARG:HG3	1:A:422:VAL:HG11	2.01	0.42
1:A:408:LEU:HD11	1:A:420:ALA:HB1	2.01	0.42
1:C:253:MSE:O	1:C:257:VAL:HG13	2.20	0.42
1:F:132:SER:O	1:F:133:SER:C	2.63	0.42
1:F:289:PHE:O	1:F:290:ASP:C	2.62	0.42
1:F:292:ILE:HG21	1:F:299:LEU:HG	2.01	0.42
1:C:36:ASN:O	1:C:37:SER:C	2.63	0.42
1:D:12:PHE:HE1	1:D:116:LEU:HD12	1.84	0.42
1:D:18:ASP:CG	1:D:54:SER:OG	2.63	0.42
1:D:285:ASP:OD1	1:D:285:ASP:C	2.62	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:24:LEU:C	1:B:24:LEU:CD2	2.92	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:C:219:PHE:O	1:C:220:GLY:C	2.62	0.42
1:D:130:LEU:C	1:D:130:LEU:HD23	2.45	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:223:THR:O	1:A:224:PRO:C	2.61	0.42
1:A:367:GLU:CG	1:A:407:VAL:HG12	2.50	0.42
1:B:53:VAL:HA	1:B:99:MSE:HE3	2.02	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:D:78:HIS:HA	1:D:79:THR:HA	1.74	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:F:365:LEU:HB3	1:F:390:THR:HG23	2.02	0.42
1:F:384:GLU:O	1:F:385:ALA:C	2.62	0.42
1:B:63:CYS:O	1:B:64:ALA:C	2.63	0.42
1:C:252:ALA:O	1:C:253:MSE:C	2.61	0.42
1:C:366:PRO:O	1:C:367:GLU:C	2.62	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:248:VAL:O	1:A:249:GLY:C	2.63	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:C:404:GLN:CB	1:F:43:SER:O	2.68	0.42
1:E:63:CYS:O	1:E:64:ALA:C	2.63	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:F:127:GLY:O	1:F:128:THR:C	2.63	0.42
1:A:31:VAL:HG12	1:A:35:LEU:CD2	2.48	0.42
1:A:299:LEU:C	1:A:299:LEU:HD22	2.45	0.42
1:A:313:PRO:O	1:A:314:LYS:C	2.63	0.42
1:B:63:CYS:HB2	1:B:68:PHE:CD2	2.55	0.42
1:B:265:VAL:HG11	1:B:292:ILE:HD13	2.01	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:350:ILE:O	1:E:354:LEU:HB2	2.20	0.42
1:A:122:LEU:HD12	1:A:122:LEU:N	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:D:17:ALA:HB3	1:D:52:ASP:CG	2.45	0.41
1:E:215:GLY:C	1:E:216:VAL:HG23	2.45	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:66:PHE:CD1	2:A:501:TLA:O41	2.74	0.41
1:A:312:GLY:HA3	1:A:332:GLN:O	2.20	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:C:390:THR:H	1:C:390:THR:HG1	1.46	0.41
1:F:124:GLY:CA	1:F:149:THR:OG1	2.68	0.41
1:A:241:LEU:HD21	1:B:177:ASN:ND2	2.35	0.41
1:A:253:MSE:O	1:A:257:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ALA:O	1:A:377:GLY:N	2.53	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:O	1:C:327:HIS:HD2	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:30:His:O	1:C:31:VAL:C	2.62	0.41
1:C:278:VAL:O	1:C:278:VAL:CG1	2.67	0.41
1:E:14:ILE:CG1	1:E:51:VAL:HG13	2.48	0.41
1:E:371:SER:N	1:E:412:ILE:HG21	2.34	0.41
1:A:241:LEU:HD21	1:B:177:ASN:CG	2.45	0.41
1:A:317:ILE:O	1:A:318:PRO:C	2.63	0.41
1:D:66:PHE:C	1:D:67:ASP:O	2.58	0.41
1:D:370:VAL:C	1:D:412:ILE:HG21	2.46	0.41
1:E:241:LEU:HD21	1:F:177:ASN:ND2	2.36	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:F:277:VAL:CG2	1:F:278:VAL:N	2.83	0.41
1:F:286:SER:O	1:F:353:LYS:NZ	2.52	0.41
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.75	0.41
1:B:58:LYS:HD3	1:B:59:GLU:N	2.35	0.41
1:B:343:ASN:HA	1:B:346:PHE:CD2	2.56	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:305:ALA:CB	1:B:308:MSE:HE3	2.47	0.41
1:B:306:LEU:HD13	1:B:306:LEU:HA	1.91	0.41
1:D:35:LEU:HD12	1:D:35:LEU:HA	1.77	0.41
1:D:252:ALA:O	1:D:256:LEU:HG	2.21	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:HA	1:A:354:LEU:HD13	1.82	0.41
1:B:340:VAL:HG21	1:B:384:GLU:OE2	2.21	0.41
1:C:271:THR:HB	1:C:305:ALA:CB	2.49	0.41
1:C:382:ASP:OD2	1:C:385:ALA:CB	2.59	0.41
1:D:130:LEU:C	1:D:130:LEU:CD2	2.93	0.41
1:D:223:THR:N	1:D:224:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:391:ARG:O	1:E:392:GLU:C	2.63	0.41
1:F:41:LYS:HA	1:F:42:SER:CB	2.50	0.41
1:F:261:PHE:C	1:F:263:GLN:HE22	2.29	0.41
1:F:275:ASP:CA	1:F:309:VAL:HG13	2.50	0.41
1:F:277:VAL:CG2	1:F:278:VAL:HG23	2.51	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: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:53:VAL:C	1:B:99:MSE:HE3	2.46	0.41
1:B:70:PRO:HD2	1:B:73:ASP:OD2	2.21	0.41
1:B:177:ASN:HD21	1:B:179:VAL:HB	1.85	0.41
1:D:69:VAL:HG23	1:D:70:PRO:N	2.36	0.41
1:E:262:ILE:C	1:E:263:GLN:HE21	2.29	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
1:C:35:LEU:HD12	1:C:35:LEU:HA	1.95	0.40
1:C:241:LEU:HD12	1:C:262:ILE:CD1	2.43	0.40
1:C:354:LEU:HD12	1:C:354:LEU:HA	1.92	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:A:112:ASP:C	1:A:114:GLN:H	2.28	0.40
1:B:307:ASP:OD1	1:B:308:MSE:HE2	2.22	0.40
1:B:390:THR:CG2	1:B:407:VAL:HG22	2.52	0.40
1:B:404:GLN:CG	1:B:405:VAL:N	2.84	0.40
1:D:414:ASP:O	1:D:415:ALA:C	2.61	0.40
1:F:303:VAL:HG23	1:F:370:VAL:HG12	2.03	0.40
1:A:14:ILE:HG23	1:A:51:VAL:CG2	2.38	0.40
1:A:113:GLU:CB	1:A:115:ASN:ND2	2.84	0.40
1:E:18:ASP:OD1	1:E:19:THR:HG22	2.22	0.40
1:E:145:VAL:HG12	1:E:146:ILE:N	2.37	0.40
1:E:412:ILE:CG2	1:E:413:ASN:N	2.84	0.40
1:F:25:ARG:O	1:F:26:PHE:C	2.64	0.40
1:F:263:GLN:NE2	1:F:263:GLN:N	2.69	0.40
1:A:91:ILE:N	1:A:91:ILE:CD1	2.70	0.40
1:A:229:VAL:HG13	1:A:422:VAL:CG2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ASP:O	1:C:424:SER:C	2.64	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:232:ARG:CG	1:E:422:VAL:HG11	2.51	0.40
1:E:307:ASP:OD2	1:E:371:SER:HB3	2.21	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 [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	400/431 (93%)	343 (86%)	45 (11%)	12 (3%)	3	7
1	B	398/431 (92%)	337 (85%)	55 (14%)	6 (2%)	8	20
1	C	392/431 (91%)	311 (79%)	56 (14%)	25 (6%)	1	1
1	D	393/431 (91%)	326 (83%)	52 (13%)	15 (4%)	2	5
1	E	377/431 (88%)	315 (84%)	52 (14%)	10 (3%)	4	9
1	F	372/431 (86%)	296 (80%)	59 (16%)	17 (5%)	2	3
All	All	2332/2586 (90%)	1928 (83%)	319 (14%)	85 (4%)	2	5

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
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

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Mol	Chain	Res	Type
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
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 [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

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 oligosaccharides 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	B	501	-	9,9,9	1.17	0	12,12,12	1.61	3 (25%)
2	TLA	A	501	-	9,9,9	1.28	1 (11%)	12,12,12	1.04	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	B	501	-	-	10/12/12/12	-
2	TLA	A	501	-	-	6/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TLA	O41-C4	-2.11	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	TLA	O2-C2-C3	-2.85	104.37	110.17
2	B	501	TLA	O41-C4-C3	2.33	119.78	113.31
2	B	501	TLA	O11-C1-O1	-2.15	119.21	124.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TLA	O2-C2-C3-O3
2	A	501	TLA	C1-C2-C3-C4
2	B	501	TLA	O3-C3-C4-O4
2	B	501	TLA	O3-C3-C4-O41
2	A	501	TLA	C1-C2-C3-O3
2	A	501	TLA	O2-C2-C3-C4
2	B	501	TLA	O11-C1-C2-C3
2	B	501	TLA	O2-C2-C3-C4
2	B	501	TLA	O2-C2-C3-O3
2	B	501	TLA	C1-C2-C3-O3
2	B	501	TLA	O11-C1-C2-O2
2	A	501	TLA	O1-C1-C2-C3
2	A	501	TLA	O11-C1-C2-C3
2	B	501	TLA	O1-C1-C2-O2
2	B	501	TLA	O1-C1-C2-C3
2	B	501	TLA	C1-C2-C3-C4

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, 95th 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 ²)	Q<0.9
1	A	397/431 (92%)	-0.08	4 (1%) 79 78	20, 56, 97, 121	0
1	B	395/431 (91%)	0.13	5 (1%) 75 73	24, 65, 111, 128	1 (0%)
1	C	392/431 (90%)	0.10	9 (2%) 61 58	28, 58, 107, 140	0
1	D	393/431 (91%)	-0.03	4 (1%) 79 78	27, 55, 98, 125	0
1	E	378/431 (87%)	0.30	19 (5%) 34 31	25, 74, 115, 135	1 (0%)
1	F	372/431 (86%)	0.42	14 (3%) 44 40	30, 78, 115, 166	0
All	All	2327/2586 (89%)	0.14	55 (2%) 59 56	20, 63, 109, 166	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	TRP	4.8
1	B	412	ILE	4.3
1	A	57	TRP	4.0
1	C	40	ASN	3.6
1	F	212	PHE	3.6
1	C	311	PHE	3.3
1	E	57	TRP	3.2
1	A	79	THR	3.2
1	F	96	ILE	3.2
1	F	123	GLY	3.2
1	C	57	TRP	3.1
1	E	219	PHE	3.0
1	E	298	PRO	3.0
1	E	380	PHE	2.8
1	C	62	SER	2.8
1	E	264	GLY	2.7
1	E	73	ASP	2.7
1	F	300	VAL	2.7
1	B	227	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	265	VAL	2.5
1	F	340	VAL	2.5
1	A	335	LEU	2.4
1	F	94	LEU	2.4
1	C	44	PHE	2.4
1	C	64	ALA	2.4
1	E	335	LEU	2.4
1	D	20	LYS	2.4
1	C	394	GLN	2.4
1	F	349	PHE	2.4
1	D	399	ASN	2.3
1	F	417	PHE	2.3
1	F	335	LEU	2.3
1	C	345	LYS	2.3
1	E	160	GLY	2.3
1	E	312	GLY	2.3
1	E	373	LEU	2.3
1	F	277	VAL	2.3
1	A	326	ILE	2.2
1	B	57	TRP	2.2
1	E	376	PRO	2.2
1	F	267	ASP	2.2
1	F	103	LEU	2.2
1	E	281	VAL	2.2
1	E	397	LEU	2.2
1	F	273	VAL	2.2
1	E	274	ALA	2.1
1	E	313	PRO	2.1
1	C	335	LEU	2.1
1	E	354	LEU	2.1
1	D	376	PRO	2.1
1	E	88	PHE	2.1
1	F	17	ALA	2.1
1	B	407	VAL	2.1
1	E	311	PHE	2.1
1	B	61	ASN	2.1

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 [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	TLA	A	501	10/10	0.85	0.09	72,74,80,86	0
2	TLA	B	501	10/10	0.86	0.11	75,85,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.