Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 10:53 AM EDT

PDB ID	:	3E0J
Title	:	X-ray structure of the complex of regulatory subunits of human DNA polymerase delta
Authors	:	Baranovskiy, A.G.; Babayeva, N.D.; Pavlov, Y.I.; Vassylyev, D.G.; Tahirov, T.H.
Deposited on	:	2008-07-31
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

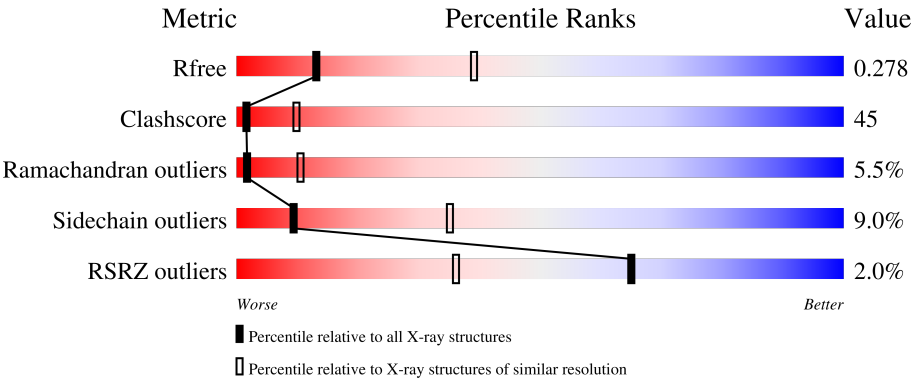
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	476	31% 48% 8% 13%
1	C	476	29% 49% 7% 14%
1	E	476	30% 47% 7% 14%
1	G	476	34% 45% 7% 14%
2	B	144	42% 50% 7%

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Mol	Chain	Length	Quality of chain
2	D	144	2% 44% 49% 6%
2	F	144	% 43% 51% 6%
2	H	144	3% 42% 52% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17153 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 DNA polymerase subunit delta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3185	2022	537	609	17			
1	C	409	Total	C	N	O	S	0	0	0
			3133	1991	530	595	17			
1	E	408	Total	C	N	O	S	0	0	0
			3125	1985	529	594	17			
1	G	408	Total	C	N	O	S	0	0	0
			3125	1985	529	594	17			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP P49005
A	-5	HIS	-	expression tag	UNP P49005
A	-4	HIS	-	expression tag	UNP P49005
A	-3	HIS	-	expression tag	UNP P49005
A	-2	HIS	-	expression tag	UNP P49005
A	-1	HIS	-	expression tag	UNP P49005
A	0	GLY	-	expression tag	UNP P49005
C	-6	HIS	-	expression tag	UNP P49005
C	-5	HIS	-	expression tag	UNP P49005
C	-4	HIS	-	expression tag	UNP P49005
C	-3	HIS	-	expression tag	UNP P49005
C	-2	HIS	-	expression tag	UNP P49005
C	-1	HIS	-	expression tag	UNP P49005
C	0	GLY	-	expression tag	UNP P49005
E	-6	HIS	-	expression tag	UNP P49005
E	-5	HIS	-	expression tag	UNP P49005
E	-4	HIS	-	expression tag	UNP P49005
E	-3	HIS	-	expression tag	UNP P49005
E	-2	HIS	-	expression tag	UNP P49005
E	-1	HIS	-	expression tag	UNP P49005
E	0	GLY	-	expression tag	UNP P49005

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	HIS	-	expression tag	UNP P49005
G	-5	HIS	-	expression tag	UNP P49005
G	-4	HIS	-	expression tag	UNP P49005
G	-3	HIS	-	expression tag	UNP P49005
G	-2	HIS	-	expression tag	UNP P49005
G	-1	HIS	-	expression tag	UNP P49005
G	0	GLY	-	expression tag	UNP P49005

- Molecule 2 is a protein called DNA polymerase subunit delta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			
2	D	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			
2	F	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			
2	H	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			

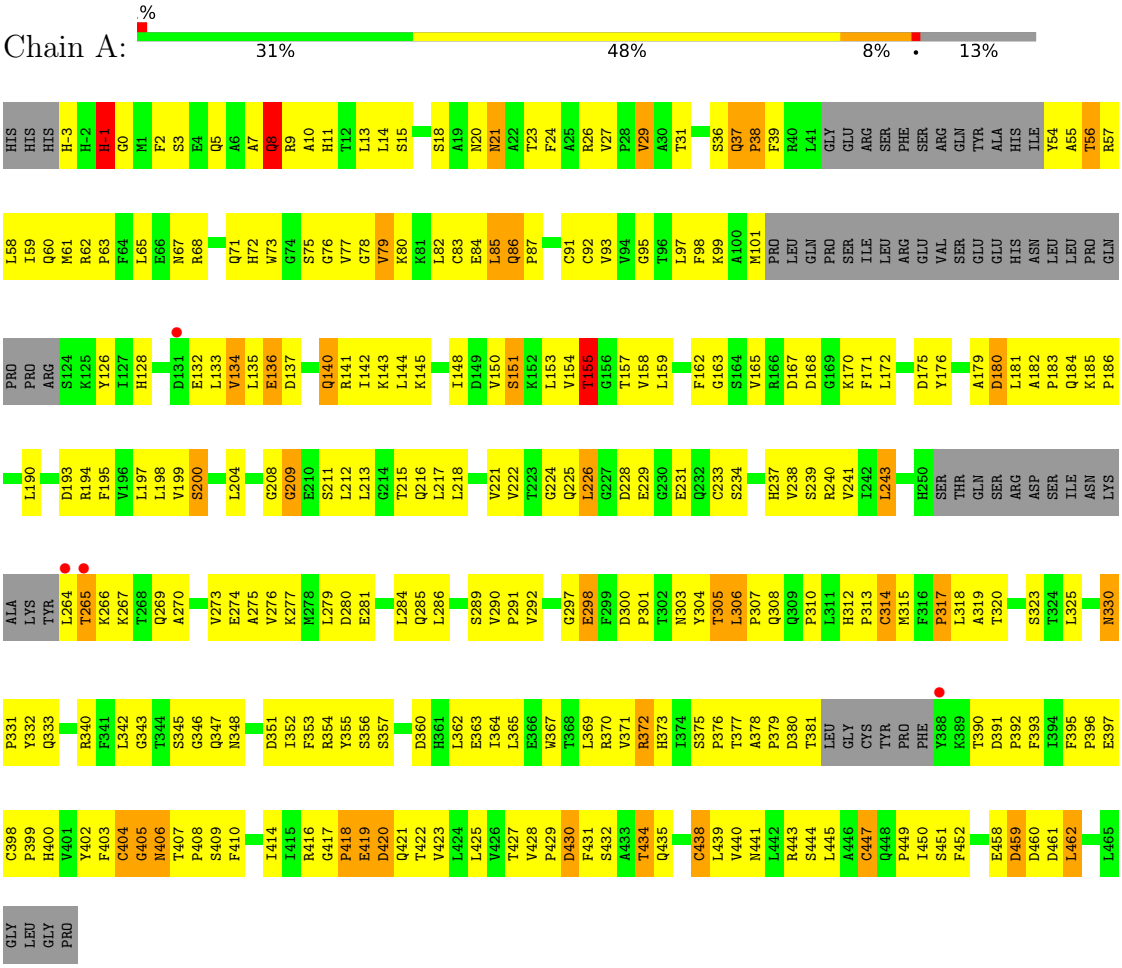
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	6	Total	O	0	0
			6	6		
3	C	12	Total	O	0	0
			12	12		
3	D	4	Total	O	0	0
			4	4		
3	E	15	Total	O	0	0
			15	15		
3	F	4	Total	O	0	0
			4	4		
3	G	8	Total	O	0	0
			8	8		
3	H	1	Total	O	0	0
			1	1		

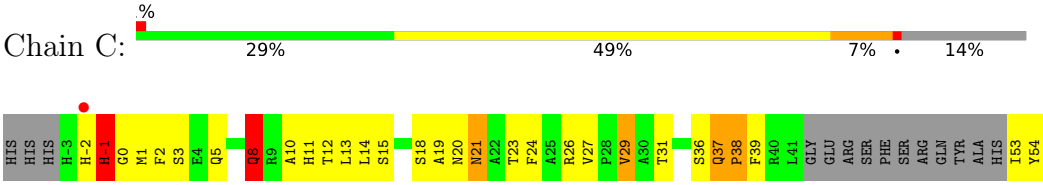
3 Residue-property plots (i)

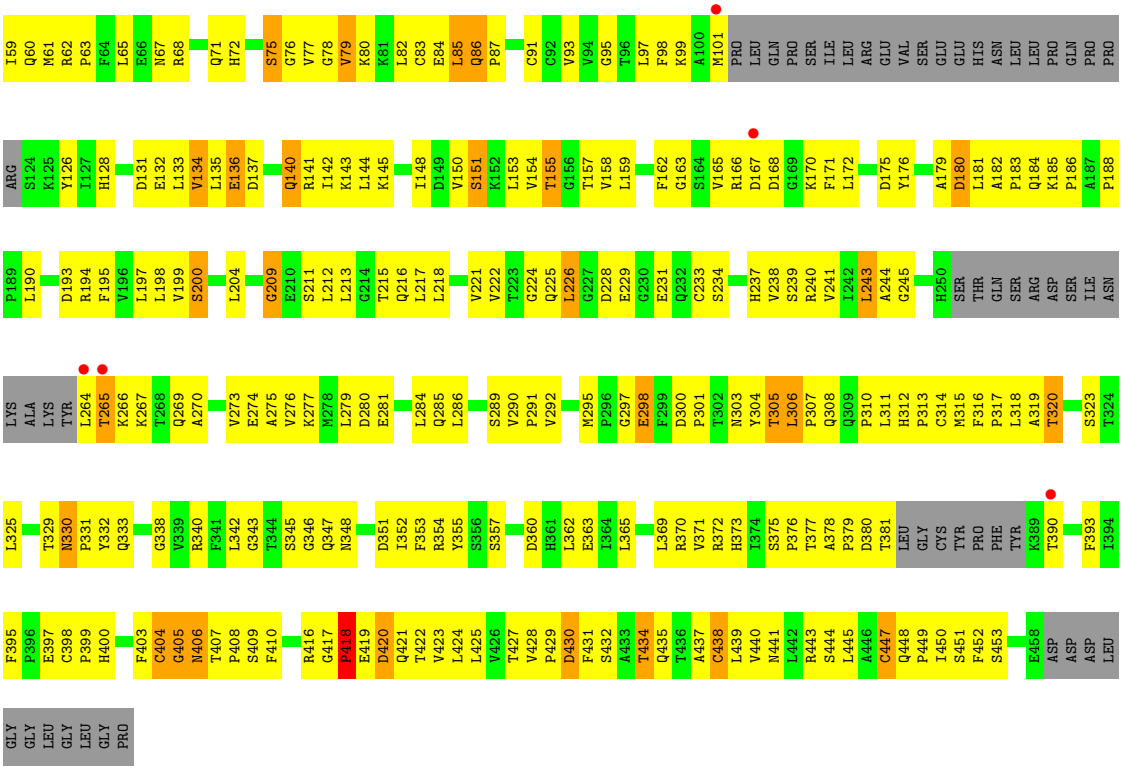
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase subunit delta-2



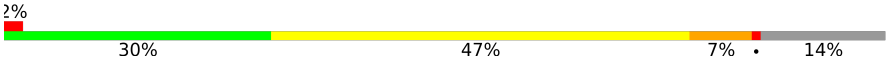
• Molecule 1: DNA polymerase subunit delta-2

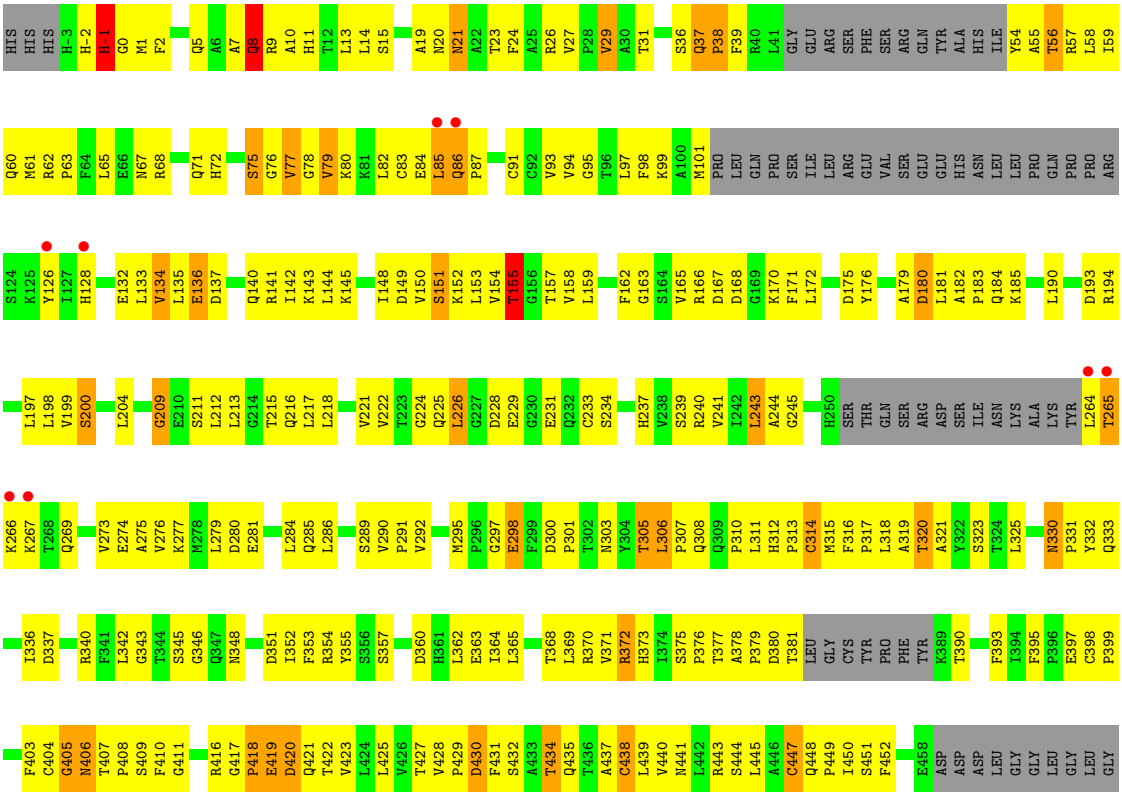




• Molecule 1: DNA polymerase subunit delta-2

Chain E:

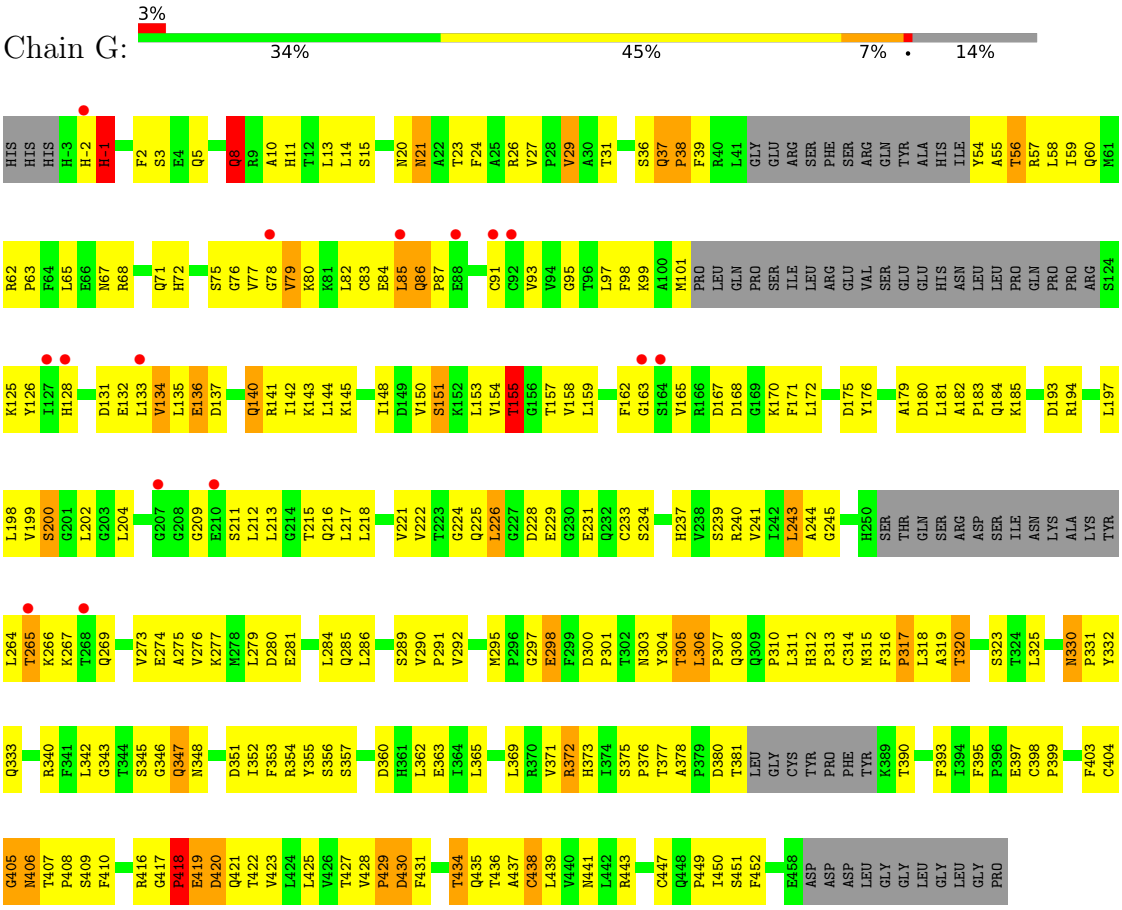




PRO

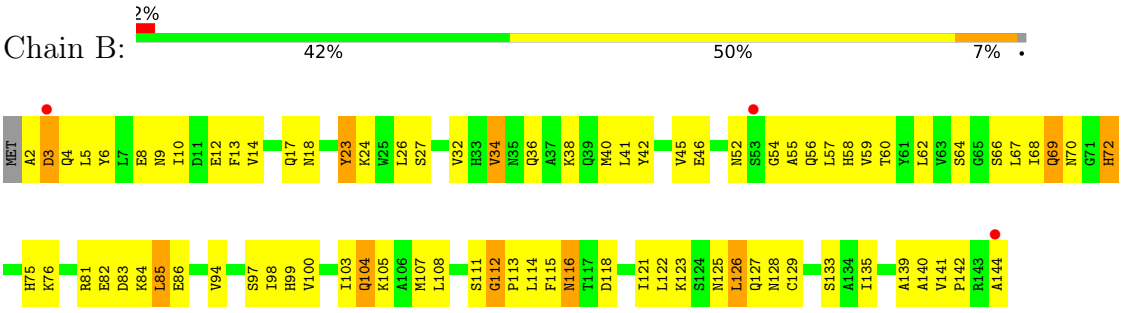
• Molecule 1: DNA polymerase subunit delta-2

Chain G:



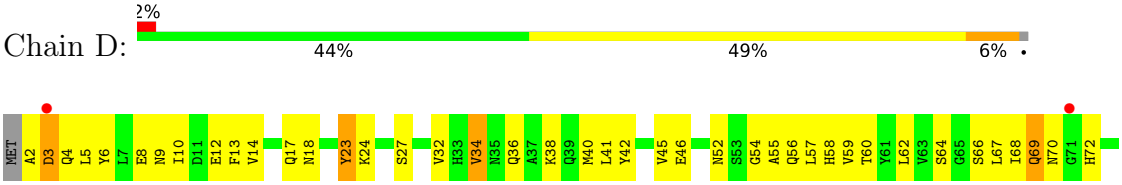
• Molecule 2: DNA polymerase subunit delta-3

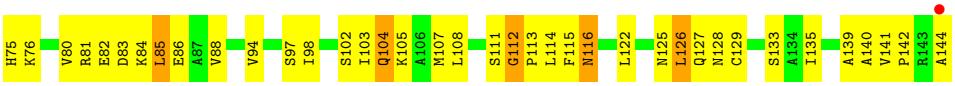
Chain B:



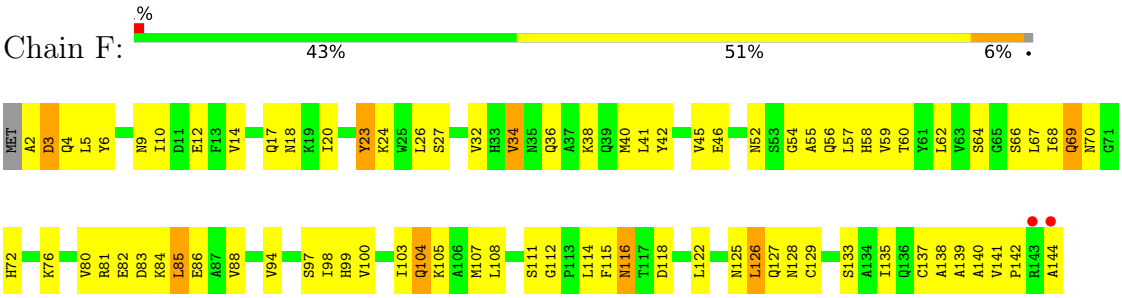
• Molecule 2: DNA polymerase subunit delta-3

Chain D:

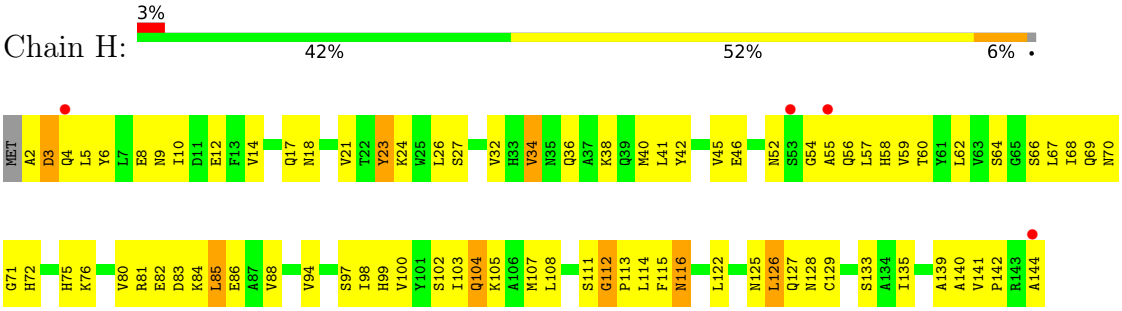




• Molecule 2: DNA polymerase subunit delta-3



• Molecule 2: DNA polymerase subunit delta-3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.13Å 248.53Å 103.46Å 90.00° 106.94° 90.00°	Depositor
Resolution (Å)	29.89 – 3.00 38.01 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.3 (29.89-3.00) 91.1 (38.01-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	123.02 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.281 0.256 , 0.278	Depositor DCC
R_{free} test set	4249 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	17153	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.54	1/3254 (0.0%)	0.78	1/4426 (0.0%)
1	C	0.56	1/3201 (0.0%)	0.78	1/4354 (0.0%)
1	E	0.53	0/3193	0.77	0/4343
1	G	0.52	0/3193	0.77	0/4343
2	B	0.56	0/1150	0.69	0/1553
2	D	0.54	0/1150	0.70	0/1553
2	F	0.51	0/1150	0.67	0/1553
2	H	0.47	0/1150	0.66	0/1553
All	All	0.54	2/17441 (0.0%)	0.75	2/23678 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	404	CYS	CB-SG	-6.43	1.71	1.82
1	A	404	CYS	CB-SG	-5.54	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	SER	N-CA-C	-5.32	96.64	111.00
1	C	18	SER	N-CA-C	-5.04	97.41	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3185	0	3150	319	0
1	C	3133	0	3112	330	0
1	E	3125	0	3101	318	0
1	G	3125	0	3101	309	0
2	B	1131	0	1138	93	0
2	D	1131	0	1138	90	0
2	F	1131	0	1138	78	0
2	H	1131	0	1138	89	0
3	A	11	0	0	1	0
3	B	6	0	0	0	0
3	C	12	0	0	3	0
3	D	4	0	0	0	0
3	E	15	0	0	2	0
3	F	4	0	0	0	0
3	G	8	0	0	2	0
3	H	1	0	0	0	0
All	All	17153	0	17016	1525	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1525) 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:C:29:VAL:HG11	1:C:291:PRO:HG2	1.19	1.18
1:C:58:LEU:HD21	1:C:95:GLY:HA2	1.25	1.13
1:E:58:LEU:HD21	1:E:95:GLY:HA2	1.25	1.09
1:A:58:LEU:HD21	1:A:95:GLY:HA2	1.26	1.09
1:G:29:VAL:HG11	1:G:291:PRO:HG2	1.24	1.09
1:G:58:LEU:HD21	1:G:95:GLY:HA2	1.29	1.09
1:A:29:VAL:HG11	1:A:291:PRO:HG2	1.12	1.07
1:E:29:VAL:HG11	1:E:291:PRO:HG2	1.21	1.07
1:G:193:ASP:HB3	1:G:443:ARG:NH1	1.74	1.00
1:C:193:ASP:HB3	1:C:443:ARG:NH1	1.80	0.97
1:A:193:ASP:HB3	1:A:443:ARG:NH1	1.81	0.94
1:G:330:ASN:HB3	1:G:331:PRO:HD3	1.50	0.94
1:C:330:ASN:HB3	1:C:331:PRO:HD3	1.48	0.94
1:G:98:PHE:HB2	1:G:134:VAL:HG13	1.51	0.92
1:C:193:ASP:HB3	1:C:443:ARG:HH11	1.33	0.91
1:E:330:ASN:HB3	1:E:331:PRO:HD3	1.49	0.91
2:B:116:ASN:HD22	2:B:116:ASN:H	1.17	0.90
2:F:116:ASN:H	2:F:116:ASN:HD22	1.20	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:ASP:HB3	1:E:443:ARG:NH1	1.86	0.89
1:A:330:ASN:HB3	1:A:331:PRO:HD3	1.55	0.89
1:E:99:LYS:H	1:E:155:THR:HG23	1.38	0.89
1:A:340:ARG:HH12	1:A:397:GLU:HB3	1.38	0.89
1:G:99:LYS:H	1:G:155:THR:HG23	1.39	0.88
1:A:193:ASP:HB3	1:A:443:ARG:HH11	1.34	0.88
1:A:98:PHE:HB2	1:A:134:VAL:HG13	1.53	0.88
1:A:407:THR:HG22	1:A:409:SER:H	1.37	0.87
1:C:99:LYS:H	1:C:155:THR:HG23	1.40	0.87
1:C:340:ARG:HH12	1:C:397:GLU:HB3	1.39	0.87
1:C:98:PHE:HB2	1:C:134:VAL:HG13	1.56	0.87
2:H:116:ASN:H	2:H:116:ASN:HD22	1.22	0.87
1:G:193:ASP:HB3	1:G:443:ARG:HH11	1.31	0.86
1:C:407:THR:HG22	1:C:409:SER:H	1.39	0.86
1:E:98:PHE:HB2	1:E:134:VAL:HG13	1.57	0.86
1:E:182:ALA:HB1	1:E:183:PRO:HD2	1.58	0.86
1:A:290:VAL:HG22	1:A:291:PRO:HD2	1.57	0.86
1:A:99:LYS:H	1:A:155:THR:HG23	1.39	0.86
1:A:29:VAL:CG1	1:A:291:PRO:HG2	2.03	0.85
1:G:340:ARG:HH12	1:G:397:GLU:HB3	1.39	0.85
1:A:182:ALA:HB1	1:A:183:PRO:HD2	1.58	0.85
1:C:193:ASP:CB	1:C:441:ASN:HD21	1.90	0.85
1:G:407:THR:HG22	1:G:409:SER:H	1.42	0.84
1:C:182:ALA:HB1	1:C:183:PRO:HD2	1.56	0.84
2:D:116:ASN:HD22	2:D:116:ASN:H	1.20	0.84
1:G:39:PHE:CE2	1:G:331:PRO:HB2	2.12	0.84
1:E:340:ARG:HH12	1:E:397:GLU:HB3	1.40	0.83
1:C:323:SER:HA	2:D:144:ALA:HB3	1.61	0.83
1:G:182:ALA:HB1	1:G:183:PRO:HD2	1.58	0.83
2:B:116:ASN:N	2:B:116:ASN:HD22	1.72	0.83
1:E:82:LEU:HD11	1:E:142:ILE:CG2	2.09	0.83
1:E:406:ASN:HD22	1:E:406:ASN:N	1.76	0.83
2:F:116:ASN:N	2:F:116:ASN:HD22	1.75	0.82
1:A:323:SER:HA	2:B:144:ALA:HB3	1.59	0.82
1:E:407:THR:HG22	1:E:409:SER:H	1.44	0.82
1:G:145:LYS:HE3	1:G:170:LYS:HB2	1.61	0.82
1:E:39:PHE:CE2	1:E:331:PRO:HB2	2.15	0.82
1:E:193:ASP:CB	1:E:441:ASN:HD21	1.93	0.81
2:D:116:ASN:HD22	2:D:116:ASN:N	1.74	0.81
1:E:145:LYS:HE3	1:E:170:LYS:HB2	1.63	0.81
1:G:82:LEU:HD21	1:G:142:ILE:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LEU:HD11	1:G:142:ILE:CG2	2.11	0.80
1:A:56:THR:HA	1:A:59:ILE:HD12	1.64	0.80
1:C:406:ASN:N	1:C:406:ASN:HD22	1.80	0.80
1:C:82:LEU:HD11	1:C:142:ILE:CG2	2.11	0.80
1:G:406:ASN:HD22	1:G:406:ASN:N	1.79	0.80
1:G:323:SER:HA	2:H:144:ALA:HB3	1.62	0.80
1:G:308:GLN:HB2	1:G:330:ASN:HB2	1.64	0.79
1:A:82:LEU:HD11	1:A:142:ILE:CG2	2.11	0.79
1:G:62:ARG:HB3	1:G:63:PRO:HD3	1.64	0.79
1:E:193:ASP:HB3	1:E:443:ARG:HH11	1.41	0.79
1:A:148:ILE:HG13	1:A:176:TYR:CE2	2.17	0.79
1:A:193:ASP:CB	1:A:441:ASN:HD21	1.95	0.79
1:A:308:GLN:HB2	1:A:330:ASN:HB2	1.62	0.79
1:E:193:ASP:O	1:E:194:ARG:HD3	1.81	0.79
1:A:62:ARG:HB3	1:A:63:PRO:HD3	1.64	0.79
1:C:308:GLN:HB2	1:C:330:ASN:HB2	1.63	0.79
1:E:151:SER:HB2	1:E:357:SER:HB2	1.65	0.79
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.65	0.79
1:A:419:GLU:O	1:A:421:GLN:HG3	1.83	0.79
1:G:56:THR:HA	1:G:59:ILE:HD12	1.64	0.79
2:B:116:ASN:H	2:B:116:ASN:ND2	1.82	0.78
1:C:145:LYS:HE3	1:C:170:LYS:HB2	1.64	0.78
1:C:330:ASN:HB3	1:C:331:PRO:CD	2.12	0.78
1:E:439:LEU:CD1	1:E:450:ILE:HD11	2.14	0.78
1:G:37:GLN:HE21	1:G:38:PRO:HD2	1.48	0.78
1:A:193:ASP:O	1:A:194:ARG:HD3	1.84	0.78
1:C:193:ASP:HB3	1:C:441:ASN:HD21	1.47	0.78
1:C:439:LEU:CD1	1:C:450:ILE:HD11	2.13	0.78
1:A:193:ASP:HB3	1:A:441:ASN:HD21	1.48	0.78
1:G:193:ASP:CB	1:G:441:ASN:HD21	1.95	0.78
2:H:116:ASN:N	2:H:116:ASN:HD22	1.78	0.78
1:A:54:TYR:HA	1:A:380:ASP:OD1	1.83	0.78
1:A:226:LEU:HD22	2:B:62:LEU:HD11	1.64	0.78
1:E:29:VAL:CG1	1:E:291:PRO:HG2	2.11	0.78
1:E:323:SER:HA	2:F:144:ALA:HB3	1.64	0.78
1:C:56:THR:HA	1:C:59:ILE:HD12	1.66	0.78
1:A:39:PHE:CE2	1:A:331:PRO:HB2	2.18	0.77
1:E:306:LEU:HB3	1:E:307:PRO:HD3	1.66	0.77
1:G:330:ASN:HB3	1:G:331:PRO:CD	2.14	0.77
1:G:54:TYR:HA	1:G:380:ASP:OD1	1.85	0.77
1:E:159:LEU:H	1:E:159:LEU:HD23	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:N	1:A:406:ASN:HD22	1.82	0.77
1:C:62:ARG:HB3	1:C:63:PRO:HD3	1.65	0.77
1:C:217:LEU:O	1:C:221:VAL:HG23	1.84	0.77
1:A:226:LEU:HD12	1:A:226:LEU:C	2.04	0.77
1:A:145:LYS:HE3	1:A:170:LYS:HB2	1.67	0.77
1:E:193:ASP:HB3	1:E:441:ASN:HD21	1.48	0.77
1:C:82:LEU:HD21	1:C:142:ILE:H	1.47	0.76
1:C:148:ILE:HG13	1:C:176:TYR:CE2	2.20	0.76
1:G:439:LEU:CD1	1:G:450:ILE:HD11	2.15	0.76
1:A:303:ASN:HD22	1:A:305:THR:CG2	1.97	0.76
1:C:29:VAL:CG1	1:C:291:PRO:HG2	2.09	0.76
1:E:82:LEU:HD21	1:E:142:ILE:H	1.51	0.76
1:E:308:GLN:HB2	1:E:330:ASN:HB2	1.67	0.76
1:G:148:ILE:HG13	1:G:176:TYR:CE2	2.19	0.76
1:E:226:LEU:HD22	2:F:62:LEU:HD11	1.66	0.76
1:E:330:ASN:HB3	1:E:331:PRO:CD	2.14	0.76
1:G:290:VAL:HG22	1:G:291:PRO:HD2	1.67	0.76
1:C:290:VAL:HG22	1:C:291:PRO:HD2	1.67	0.76
1:G:306:LEU:HB3	1:G:307:PRO:HD3	1.68	0.76
1:C:419:GLU:O	1:C:421:GLN:HG3	1.85	0.75
2:F:116:ASN:H	2:F:116:ASN:ND2	1.83	0.75
1:G:419:GLU:O	1:G:421:GLN:HG3	1.86	0.75
1:E:148:ILE:HG13	1:E:176:TYR:CE2	2.22	0.75
1:C:39:PHE:CE2	1:C:331:PRO:HB2	2.20	0.75
2:D:116:ASN:ND2	2:D:116:ASN:H	1.85	0.75
1:E:56:THR:HA	1:E:59:ILE:HD12	1.67	0.75
1:G:95:GLY:HA3	1:G:135:LEU:HD11	1.68	0.75
1:A:37:GLN:HE21	1:A:38:PRO:HD2	1.52	0.75
1:C:193:ASP:O	1:C:194:ARG:HD3	1.87	0.75
1:A:82:LEU:HD21	1:A:142:ILE:H	1.50	0.75
1:E:37:GLN:HE21	1:E:38:PRO:HD2	1.52	0.75
1:G:217:LEU:O	1:G:221:VAL:HG23	1.87	0.75
1:E:419:GLU:O	1:E:421:GLN:HG3	1.85	0.74
1:G:303:ASN:HD22	1:G:305:THR:CG2	1.99	0.74
1:E:290:VAL:HG22	1:E:291:PRO:HD2	1.66	0.74
1:A:151:SER:HB2	1:A:357:SER:HB2	1.69	0.74
1:C:303:ASN:HD22	1:C:305:THR:CG2	2.00	0.74
2:B:66:SER:HB3	2:B:94:VAL:HG12	1.70	0.74
1:A:82:LEU:HD11	1:A:142:ILE:HG21	1.70	0.74
1:A:330:ASN:HB3	1:A:331:PRO:CD	2.18	0.74
1:C:226:LEU:HD22	2:D:62:LEU:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ASP:O	1:G:194:ARG:HD3	1.86	0.74
1:E:82:LEU:HD11	1:E:142:ILE:HG21	1.68	0.73
1:C:37:GLN:HE21	1:C:38:PRO:HD2	1.52	0.73
1:C:82:LEU:HD11	1:C:142:ILE:HG21	1.70	0.73
1:C:333:GLN:HG2	1:C:342:LEU:HD13	1.71	0.73
1:A:29:VAL:HG11	1:A:291:PRO:CG	2.07	0.73
1:A:330:ASN:O	1:A:331:PRO:C	2.26	0.73
1:E:95:GLY:HA3	1:E:135:LEU:HD11	1.71	0.73
2:F:85:LEU:O	2:F:85:LEU:HD12	1.88	0.73
1:G:333:GLN:HG2	1:G:342:LEU:HD13	1.70	0.73
1:A:95:GLY:HA3	1:A:135:LEU:HD11	1.69	0.72
1:E:62:ARG:HB3	1:E:63:PRO:HD3	1.70	0.72
1:A:142:ILE:HD13	1:A:171:PHE:HB2	1.69	0.72
1:G:151:SER:HB2	1:G:357:SER:HB2	1.71	0.72
1:G:184:GLN:HB2	1:G:398:CYS:HB3	1.69	0.72
1:A:77:VAL:HG13	1:A:79:VAL:HG23	1.71	0.72
1:C:151:SER:HB2	1:C:357:SER:HB2	1.71	0.72
1:G:365:LEU:HD13	1:G:404:CYS:HB2	1.71	0.72
1:G:82:LEU:HD11	1:G:142:ILE:HG21	1.70	0.72
1:G:221:VAL:HG22	1:G:226:LEU:HD11	1.72	0.72
1:G:226:LEU:C	1:G:226:LEU:HD12	2.10	0.72
1:A:439:LEU:CD1	1:A:450:ILE:HD11	2.20	0.72
1:C:54:TYR:HA	1:C:380:ASP:OD1	1.90	0.72
1:C:159:LEU:HD23	1:C:159:LEU:H	1.54	0.71
1:A:418:PRO:HB2	1:A:419:GLU:OE1	1.88	0.71
1:G:142:ILE:HD13	1:G:171:PHE:HB2	1.70	0.71
2:H:116:ASN:H	2:H:116:ASN:ND2	1.87	0.71
1:A:407:THR:HG23	1:A:408:PRO:HD2	1.71	0.71
1:G:193:ASP:HB3	1:G:441:ASN:HD21	1.54	0.71
1:A:333:GLN:HG2	1:A:342:LEU:HD13	1.72	0.71
1:E:221:VAL:HG22	1:E:226:LEU:HD11	1.72	0.71
1:E:303:ASN:HD22	1:E:305:THR:CG2	2.03	0.71
1:C:95:GLY:HA3	1:C:135:LEU:HD11	1.70	0.71
1:C:142:ILE:HD13	1:C:171:PHE:HB2	1.71	0.71
1:C:365:LEU:HD13	1:C:404:CYS:HB2	1.73	0.71
1:A:315:MET:O	1:A:317:PRO:HD3	1.92	0.70
1:A:217:LEU:O	1:A:221:VAL:HG23	1.91	0.70
2:B:85:LEU:O	2:B:85:LEU:HD12	1.90	0.70
2:D:70:ASN:H	2:D:72:HIS:CD2	2.08	0.70
1:G:75:SER:O	1:G:77:VAL:N	2.23	0.70
1:G:226:LEU:HD22	2:H:62:LEU:HD11	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:SER:O	1:C:77:VAL:N	2.24	0.70
1:A:159:LEU:H	1:A:159:LEU:HD23	1.57	0.70
1:E:226:LEU:C	1:E:226:LEU:HD12	2.12	0.70
1:C:315:MET:O	1:C:317:PRO:HD3	1.92	0.70
1:A:86:GLN:HA	1:A:86:GLN:HE21	1.57	0.69
3:C:471:HOH:O	1:E:21:ASN:HB2	1.92	0.69
1:G:29:VAL:CG1	1:G:291:PRO:HG2	2.14	0.69
1:E:418:PRO:HB2	1:E:419:GLU:OE1	1.92	0.69
1:E:54:TYR:HA	1:E:380:ASP:OD1	1.91	0.69
1:A:303:ASN:HA	1:C:303:ASN:HA	1.74	0.69
1:C:329:THR:HG23	3:C:476:HOH:O	1.91	0.69
1:A:80:LYS:HD2	1:A:84:GLU:HB2	1.74	0.69
1:A:82:LEU:O	1:A:85:LEU:HD22	1.92	0.69
1:G:333:GLN:CG	1:G:342:LEU:HD13	2.22	0.69
1:G:406:ASN:HD22	1:G:406:ASN:H	1.40	0.69
1:C:281:GLU:O	1:C:285:GLN:HG3	1.91	0.69
1:E:75:SER:O	1:E:77:VAL:N	2.26	0.69
1:E:142:ILE:HD13	1:E:171:PHE:HB2	1.73	0.69
1:G:82:LEU:O	1:G:85:LEU:HD22	1.91	0.69
1:E:27:VAL:CG1	1:E:237:HIS:HA	2.22	0.69
1:A:75:SER:O	1:A:77:VAL:N	2.25	0.69
1:G:330:ASN:O	1:G:331:PRO:C	2.28	0.69
1:G:39:PHE:CD2	1:G:331:PRO:HB2	2.27	0.69
1:G:340:ARG:NH1	1:G:397:GLU:HB3	2.08	0.69
1:C:226:LEU:C	1:C:226:LEU:HD12	2.14	0.68
1:A:58:LEU:HD21	1:A:95:GLY:CA	2.17	0.68
2:F:139:ALA:O	2:F:141:VAL:N	2.24	0.68
1:G:277:LYS:HE2	1:G:281:GLU:OE2	1.94	0.68
2:D:85:LEU:O	2:D:85:LEU:HD12	1.93	0.68
1:A:303:ASN:HD22	1:A:305:THR:HG23	1.59	0.68
1:A:65:LEU:HD21	1:A:158:VAL:O	1.94	0.68
1:E:37:GLN:HE21	1:E:38:PRO:CD	2.06	0.68
1:A:365:LEU:HD13	1:A:404:CYS:HB2	1.75	0.68
1:G:159:LEU:HD23	1:G:159:LEU:H	1.58	0.68
2:H:85:LEU:O	2:H:85:LEU:HD12	1.93	0.68
1:E:151:SER:HB2	1:E:357:SER:CB	2.24	0.68
1:C:306:LEU:HB3	1:C:307:PRO:HD3	1.76	0.68
1:E:82:LEU:O	1:E:85:LEU:HD22	1.93	0.68
1:A:340:ARG:NH1	1:A:397:GLU:HB3	2.09	0.67
1:A:77:VAL:HG13	1:A:79:VAL:CG2	2.24	0.67
1:C:133:LEU:O	1:C:144:LEU:HD12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ARG:NH1	1:C:397:GLU:HB3	2.07	0.67
1:A:37:GLN:HE21	1:A:38:PRO:CD	2.07	0.67
1:G:82:LEU:HD21	1:G:142:ILE:N	2.09	0.67
1:E:184:GLN:HB2	1:E:398:CYS:HB3	1.75	0.67
1:C:453:SER:HA	3:C:473:HOH:O	1.93	0.67
1:G:315:MET:O	1:G:317:PRO:HD3	1.93	0.67
1:A:80:LYS:CD	1:A:84:GLU:HB2	2.24	0.67
2:B:57:LEU:HD11	2:B:103:ILE:HG23	1.77	0.67
1:E:148:ILE:HA	1:E:176:TYR:HE2	1.59	0.67
1:C:181:LEU:HD12	1:C:417:GLY:HA3	1.76	0.67
1:C:82:LEU:O	1:C:85:LEU:HD22	1.95	0.67
1:E:330:ASN:O	1:E:331:PRO:C	2.28	0.67
1:E:77:VAL:HG13	1:E:79:VAL:HG23	1.76	0.67
1:G:97:LEU:HG	1:G:159:LEU:HD21	1.77	0.67
2:B:68:ILE:HD12	2:B:68:ILE:N	2.10	0.67
2:F:68:ILE:N	2:F:68:ILE:HD12	2.09	0.66
1:C:418:PRO:HB2	1:C:419:GLU:OE1	1.94	0.66
1:G:80:LYS:HD2	1:G:84:GLU:HB2	1.78	0.66
1:G:86:GLN:HE21	1:G:86:GLN:HA	1.59	0.66
1:C:86:GLN:HE21	1:C:86:GLN:HA	1.60	0.66
1:E:277:LYS:HE2	1:E:281:GLU:OE2	1.93	0.66
1:E:406:ASN:H	1:E:406:ASN:HD22	1.42	0.66
1:G:37:GLN:HE21	1:G:38:PRO:CD	2.09	0.66
1:G:77:VAL:HG13	1:G:79:VAL:HG23	1.76	0.66
1:C:303:ASN:HD22	1:C:305:THR:HG23	1.60	0.66
1:C:330:ASN:O	1:C:331:PRO:C	2.30	0.66
1:E:365:LEU:HD13	1:E:404:CYS:HB2	1.76	0.66
1:A:27:VAL:CG1	1:A:237:HIS:HA	2.25	0.66
1:E:39:PHE:CD2	1:E:331:PRO:HB2	2.30	0.66
1:G:330:ASN:O	1:G:332:TYR:N	2.29	0.66
1:G:418:PRO:HB2	1:G:419:GLU:OE1	1.95	0.66
1:G:430:ASP:O	1:G:434:THR:HG23	1.95	0.66
1:A:221:VAL:HG22	1:A:226:LEU:HD11	1.77	0.66
2:D:139:ALA:O	2:D:141:VAL:N	2.25	0.66
1:G:417:GLY:HA3	1:G:421:GLN:OE1	1.96	0.66
1:A:82:LEU:HD21	1:A:142:ILE:N	2.10	0.66
1:C:82:LEU:HD21	1:C:142:ILE:N	2.10	0.66
1:E:226:LEU:HD22	2:F:62:LEU:CD1	2.26	0.66
1:A:97:LEU:HG	1:A:159:LEU:HD21	1.77	0.66
1:E:410:PHE:HE1	1:E:438:CYS:HB2	1.61	0.66
2:F:57:LEU:HD11	2:F:103:ILE:HG23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:ALA:HB1	1:G:325:LEU:HD22	1.77	0.66
1:A:410:PHE:HE1	1:A:438:CYS:HB2	1.61	0.65
1:C:184:GLN:HB2	1:C:398:CYS:HB3	1.77	0.65
1:E:417:GLY:HA3	1:E:421:GLN:OE1	1.96	0.65
1:E:430:ASP:O	1:E:434:THR:HG23	1.96	0.65
1:A:330:ASN:O	1:A:332:TYR:N	2.30	0.65
1:G:65:LEU:HD21	1:G:158:VAL:O	1.96	0.65
1:G:303:ASN:HD22	1:G:305:THR:HG23	1.60	0.65
1:A:417:GLY:HA3	1:A:421:GLN:OE1	1.97	0.65
1:C:37:GLN:HE21	1:C:38:PRO:CD	2.08	0.65
2:D:69:GLN:HB2	2:D:72:HIS:CD2	2.31	0.65
1:A:27:VAL:HG13	1:A:237:HIS:HA	1.78	0.65
1:C:151:SER:HB2	1:C:357:SER:CB	2.27	0.65
1:C:142:ILE:CD1	1:C:171:PHE:HB2	2.26	0.65
1:G:133:LEU:O	1:G:144:LEU:HD12	1.96	0.65
1:G:37:GLN:O	1:G:39:PHE:N	2.28	0.65
1:G:407:THR:HG23	1:G:408:PRO:HD2	1.77	0.65
2:H:125:ASN:O	2:H:127:GLN:N	2.29	0.65
1:C:126:TYR:HD2	1:C:355:TYR:HE1	1.44	0.65
1:C:37:GLN:NE2	1:C:37:GLN:H	1.95	0.65
1:C:80:LYS:HD2	1:C:84:GLU:HB2	1.79	0.65
1:A:142:ILE:CD1	1:A:171:PHE:HB2	2.27	0.65
1:A:151:SER:HB2	1:A:357:SER:CB	2.27	0.65
1:E:306:LEU:O	1:E:308:GLN:N	2.30	0.64
1:G:181:LEU:HD12	1:G:417:GLY:HA3	1.79	0.64
1:G:439:LEU:HG	1:G:450:ILE:HD11	1.79	0.64
2:B:67:LEU:HD23	2:B:76:LYS:HE3	1.80	0.64
1:G:145:LYS:CE	1:G:170:LYS:HB2	2.28	0.64
1:G:209:GLY:O	1:G:212:LEU:HB2	1.97	0.64
2:H:57:LEU:HD11	2:H:103:ILE:HG23	1.77	0.64
1:A:439:LEU:HG	1:A:450:ILE:HD11	1.79	0.64
1:C:410:PHE:HE1	1:C:438:CYS:HB2	1.63	0.64
1:C:65:LEU:HD21	1:C:158:VAL:O	1.98	0.64
1:E:330:ASN:O	1:E:332:TYR:N	2.29	0.64
1:E:54:TYR:N	3:E:477:HOH:O	2.31	0.64
2:H:68:ILE:HD12	2:H:68:ILE:N	2.13	0.64
2:H:66:SER:HB3	2:H:94:VAL:HG12	1.78	0.64
1:C:277:LYS:HE2	1:C:281:GLU:OE2	1.98	0.64
1:C:406:ASN:H	1:C:406:ASN:HD22	1.45	0.64
1:C:97:LEU:HG	1:C:159:LEU:HD21	1.79	0.64
1:E:154:VAL:HG11	1:E:355:TYR:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:410:PHE:HE1	1:G:438:CYS:HB2	1.61	0.64
1:A:184:GLN:HB2	1:A:398:CYS:HB3	1.78	0.64
1:A:406:ASN:HD22	1:A:406:ASN:H	1.45	0.64
1:E:37:GLN:O	1:E:39:PHE:N	2.31	0.64
1:G:37:GLN:NE2	1:G:37:GLN:H	1.95	0.64
1:A:277:LYS:HE2	1:A:281:GLU:OE2	1.98	0.64
1:C:77:VAL:HG13	1:C:79:VAL:HG23	1.80	0.64
1:C:80:LYS:CD	1:C:84:GLU:HB2	2.28	0.64
1:G:269:GLN:O	1:G:273:VAL:HG23	1.98	0.64
1:G:77:VAL:HG13	1:G:79:VAL:CG2	2.28	0.64
1:E:77:VAL:HG13	1:E:79:VAL:CG2	2.28	0.64
1:E:80:LYS:HD2	1:E:84:GLU:HB2	1.80	0.64
1:E:86:GLN:HA	1:E:86:GLN:HE21	1.62	0.64
1:C:333:GLN:CG	1:C:342:LEU:HD13	2.27	0.63
2:D:57:LEU:HD11	2:D:103:ILE:HG23	1.80	0.63
1:G:151:SER:HB2	1:G:357:SER:CB	2.28	0.63
1:G:27:VAL:HG13	1:G:237:HIS:HA	1.81	0.63
1:E:55:ALA:O	1:E:59:ILE:HG13	1.98	0.63
1:A:37:GLN:O	1:A:39:PHE:N	2.30	0.63
2:B:12:GLU:O	2:B:17:GLN:HG3	1.98	0.63
1:C:193:ASP:HB2	1:C:441:ASN:HD21	1.63	0.63
1:G:142:ILE:CD1	1:G:171:PHE:HB2	2.28	0.63
1:G:27:VAL:CG1	1:G:237:HIS:HA	2.28	0.63
1:A:269:GLN:O	1:A:273:VAL:HG23	1.98	0.63
1:E:419:GLU:CD	1:E:419:GLU:H	2.01	0.63
1:E:82:LEU:HD21	1:E:142:ILE:N	2.12	0.63
1:A:407:THR:CG2	1:A:408:PRO:HD2	2.28	0.63
1:C:439:LEU:HG	1:C:450:ILE:HD11	1.80	0.63
2:D:69:GLN:HB2	2:D:72:HIS:NE2	2.13	0.63
1:E:303:ASN:HD22	1:E:305:THR:HG23	1.61	0.63
1:C:209:GLY:O	1:C:212:LEU:HB2	1.99	0.63
1:C:231:GLU:HG3	2:D:97:SER:OG	1.98	0.63
1:A:319:ALA:HB1	1:A:325:LEU:HD22	1.80	0.63
1:C:27:VAL:CG1	1:C:237:HIS:HA	2.28	0.63
2:B:70:ASN:H	2:B:72:HIS:CD2	2.16	0.63
1:C:430:ASP:O	1:C:434:THR:HG23	1.99	0.63
1:E:333:GLN:HG2	1:E:342:LEU:HD13	1.81	0.63
2:H:139:ALA:O	2:H:141:VAL:N	2.30	0.63
1:A:290:VAL:HG22	1:A:291:PRO:CD	2.27	0.62
1:A:333:GLN:CG	1:A:342:LEU:HD13	2.28	0.62
1:A:343:GLY:HA3	1:A:403:PHE:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD12	1:A:417:GLY:HA3	1.80	0.62
1:C:19:ALA:HB1	1:E:193:ASP:H	1.61	0.62
1:E:319:ALA:HB1	1:E:325:LEU:HD22	1.80	0.62
2:B:139:ALA:O	2:B:141:VAL:N	2.27	0.62
1:C:226:LEU:HD22	2:D:62:LEU:CD1	2.28	0.62
1:C:330:ASN:O	1:C:332:TYR:N	2.31	0.62
1:G:148:ILE:HA	1:G:176:TYR:HE2	1.63	0.62
1:G:281:GLU:O	1:G:285:GLN:HG3	1.99	0.62
1:G:80:LYS:CD	1:G:84:GLU:HB2	2.29	0.62
1:C:193:ASP:HB2	1:C:441:ASN:ND2	2.14	0.62
2:D:68:ILE:N	2:D:68:ILE:HD12	2.14	0.62
1:E:75:SER:O	1:E:77:VAL:HG23	2.00	0.62
1:E:209:GLY:O	1:E:212:LEU:HB2	2.00	0.62
1:E:27:VAL:HG13	1:E:237:HIS:HA	1.82	0.62
1:E:407:THR:HG23	1:E:408:PRO:HD2	1.80	0.62
1:G:126:TYR:HD2	1:G:355:TYR:HE1	1.47	0.62
1:E:37:GLN:NE2	1:E:38:PRO:HD2	2.15	0.62
1:C:407:THR:OG1	1:C:427:THR:HB	1.99	0.62
1:C:26:ARG:HG3	1:C:27:VAL:N	2.15	0.62
1:E:333:GLN:CG	1:E:342:LEU:HD13	2.30	0.62
2:F:66:SER:HB3	2:F:94:VAL:HG12	1.81	0.62
1:C:148:ILE:HA	1:C:176:TYR:HE2	1.65	0.62
1:G:243:LEU:HD23	1:G:243:LEU:N	2.14	0.62
1:A:419:GLU:CD	1:A:419:GLU:H	2.03	0.61
2:F:70:ASN:C	2:F:72:HIS:H	2.04	0.61
1:A:55:ALA:O	1:A:59:ILE:HG13	2.00	0.61
1:C:65:LEU:CD2	1:C:158:VAL:HG12	2.30	0.61
1:E:281:GLU:O	1:E:285:GLN:HG3	2.00	0.61
1:G:13:LEU:HD13	2:H:38:LYS:HD2	1.82	0.61
1:A:281:GLU:O	1:A:285:GLN:HG3	2.00	0.61
1:C:417:GLY:HA3	1:C:421:GLN:OE1	1.99	0.61
1:A:37:GLN:NE2	1:A:37:GLN:H	1.99	0.61
1:C:132:GLU:OE2	1:C:143:LYS:HE2	2.00	0.61
1:C:27:VAL:HG13	1:C:237:HIS:HA	1.81	0.61
1:E:133:LEU:O	1:E:144:LEU:HD12	2.00	0.61
1:E:65:LEU:HD21	1:E:158:VAL:O	2.00	0.61
1:E:340:ARG:NH1	1:E:397:GLU:HB3	2.11	0.61
1:G:65:LEU:CD2	1:G:158:VAL:HG12	2.31	0.61
1:G:226:LEU:HB2	2:H:62:LEU:CD1	2.30	0.61
1:G:343:GLY:HA3	1:G:403:PHE:CE1	2.36	0.61
1:C:55:ALA:O	1:C:59:ILE:HG13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:LEU:HD23	1:G:159:LEU:O	1.99	0.61
1:A:226:LEU:HD22	2:B:62:LEU:CD1	2.29	0.61
1:C:193:ASP:H	1:E:19:ALA:HB1	1.65	0.61
1:C:319:ALA:HB1	1:C:325:LEU:HD22	1.83	0.61
2:D:116:ASN:ND2	2:D:116:ASN:N	2.45	0.61
1:G:439:LEU:CG	1:G:450:ILE:HD11	2.31	0.61
1:C:439:LEU:CG	1:C:450:ILE:HD11	2.30	0.61
1:G:37:GLN:NE2	1:G:38:PRO:HD2	2.16	0.61
1:G:55:ALA:O	1:G:59:ILE:HG13	2.01	0.61
2:D:125:ASN:O	2:D:127:GLN:N	2.33	0.61
1:G:133:LEU:HD21	1:G:150:VAL:HG13	1.83	0.61
2:B:111:SER:O	2:B:114:LEU:HB2	2.00	0.61
1:G:290:VAL:HG22	1:G:291:PRO:CD	2.31	0.61
1:C:221:VAL:HG22	1:C:226:LEU:HD11	1.83	0.60
1:C:39:PHE:CD2	1:C:331:PRO:HB2	2.36	0.60
1:C:97:LEU:HD22	1:C:133:LEU:HB3	1.83	0.60
1:G:154:VAL:HG11	1:G:355:TYR:HB2	1.83	0.60
1:A:209:GLY:O	1:A:212:LEU:HB2	2.00	0.60
1:E:145:LYS:CE	1:E:170:LYS:HB2	2.31	0.60
1:G:406:ASN:ND2	1:G:406:ASN:N	2.50	0.60
2:H:67:LEU:HD23	2:H:76:LYS:HE3	1.82	0.60
1:A:290:VAL:CG2	1:A:291:PRO:HD2	2.31	0.60
1:A:39:PHE:CD2	1:A:331:PRO:HB2	2.37	0.60
1:E:97:LEU:HG	1:E:159:LEU:HD21	1.83	0.60
1:G:193:ASP:HB2	1:G:441:ASN:ND2	2.17	0.60
1:C:58:LEU:HD21	1:C:95:GLY:CA	2.17	0.60
1:E:315:MET:O	1:E:317:PRO:HD3	2.02	0.60
1:E:343:GLY:HA3	1:E:403:PHE:CE1	2.36	0.60
1:E:142:ILE:CD1	1:E:171:PHE:HB2	2.32	0.60
1:G:37:GLN:C	1:G:39:PHE:H	2.05	0.60
1:A:148:ILE:HA	1:A:176:TYR:HE2	1.66	0.60
1:A:126:TYR:HD2	1:A:355:TYR:HE1	1.49	0.60
1:E:68:ARG:HG3	1:E:179:ALA:HA	1.84	0.60
1:G:193:ASP:HB2	1:G:441:ASN:HD21	1.66	0.60
2:D:66:SER:HB3	2:D:94:VAL:HG12	1.83	0.60
1:A:-1:HIS:ND1	1:A:0:GLY:N	2.50	0.60
1:E:58:LEU:HD21	1:E:95:GLY:CA	2.17	0.60
1:G:226:LEU:HD22	2:H:62:LEU:CD1	2.32	0.60
1:G:306:LEU:O	1:G:308:GLN:N	2.35	0.60
2:H:116:ASN:N	2:H:116:ASN:ND2	2.48	0.60
1:C:286:LEU:HB3	1:C:292:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LEU:HD23	1:E:159:LEU:O	2.02	0.60
1:A:5:GLN:O	1:A:8:GLN:HB2	2.02	0.59
1:G:439:LEU:HG	1:G:450:ILE:CD1	2.32	0.59
1:A:226:LEU:CD1	1:A:226:LEU:C	2.70	0.59
1:C:133:LEU:HD21	1:C:150:VAL:HG13	1.84	0.59
1:A:314:CYS:SG	1:C:315:MET:HG2	2.42	0.59
1:E:193:ASP:OD2	1:E:193:ASP:N	2.34	0.59
1:E:231:GLU:HG3	2:F:97:SER:OG	2.03	0.59
1:E:193:ASP:HB2	1:E:441:ASN:ND2	2.17	0.59
2:D:70:ASN:C	2:D:72:HIS:H	2.05	0.59
1:G:380:ASP:O	1:G:381:THR:HG23	2.03	0.59
1:A:133:LEU:O	1:A:144:LEU:HD12	2.02	0.59
1:A:154:VAL:HG11	1:A:355:TYR:HB2	1.84	0.59
1:A:37:GLN:C	1:A:39:PHE:H	2.06	0.59
1:C:13:LEU:HD13	2:D:38:LYS:HD2	1.84	0.59
1:E:37:GLN:H	1:E:37:GLN:NE2	2.00	0.59
1:G:68:ARG:HG3	1:G:179:ALA:HA	1.85	0.59
2:B:66:SER:HB3	2:B:94:VAL:CG1	2.32	0.59
1:C:101:MET:HB2	1:C:128:HIS:CG	2.38	0.59
1:E:80:LYS:CD	1:E:84:GLU:HB2	2.32	0.59
1:A:430:ASP:O	1:A:434:THR:HG23	2.03	0.58
1:A:439:LEU:HG	1:A:450:ILE:CD1	2.33	0.58
2:B:125:ASN:O	2:B:127:GLN:N	2.36	0.58
1:E:82:LEU:HD11	1:E:142:ILE:HG22	1.83	0.58
1:A:348:ASN:CB	1:A:375:SER:HB2	2.32	0.58
1:A:439:LEU:CG	1:A:450:ILE:HD11	2.33	0.58
1:C:193:ASP:N	1:C:193:ASP:OD2	2.36	0.58
1:G:419:GLU:CD	1:G:419:GLU:H	2.06	0.58
1:C:407:THR:O	1:C:429:PRO:HA	2.03	0.58
1:C:77:VAL:HG13	1:C:79:VAL:CG2	2.33	0.58
1:E:217:LEU:O	1:E:221:VAL:HG23	2.03	0.58
2:F:64:SER:OG	2:F:97:SER:HB2	2.03	0.58
1:G:407:THR:CG2	1:G:408:PRO:HD2	2.33	0.58
1:A:407:THR:OG1	1:A:427:THR:HB	2.03	0.58
1:C:406:ASN:N	1:C:406:ASN:ND2	2.51	0.58
1:E:133:LEU:HD21	1:E:150:VAL:HG13	1.85	0.58
1:A:185:LYS:HE3	1:A:397:GLU:OE2	2.04	0.58
1:G:274:GLU:O	1:G:277:LYS:HB3	2.03	0.58
1:C:269:GLN:O	1:C:273:VAL:HG23	2.04	0.58
1:E:286:LEU:HB3	1:E:292:VAL:HG21	1.86	0.58
1:E:193:ASP:HB2	1:E:441:ASN:HD21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:LEU:HD22	1:E:133:LEU:HB3	1.85	0.58
1:A:97:LEU:HD22	1:A:133:LEU:HB3	1.84	0.58
1:G:26:ARG:HG3	1:G:27:VAL:N	2.18	0.58
1:G:82:LEU:HD11	1:G:142:ILE:HG22	1.85	0.58
2:F:125:ASN:O	2:F:127:GLN:N	2.37	0.58
1:A:101:MET:HB2	1:A:128:HIS:CG	2.39	0.58
1:A:226:LEU:HB2	2:B:62:LEU:CD1	2.34	0.58
1:E:274:GLU:O	1:E:277:LYS:HB3	2.04	0.58
1:E:343:GLY:HA3	1:E:403:PHE:CD1	2.39	0.58
1:A:193:ASP:HB2	1:A:441:ASN:ND2	2.19	0.58
1:C:306:LEU:HD12	1:C:306:LEU:O	2.03	0.58
1:C:419:GLU:H	1:C:419:GLU:CD	2.07	0.58
1:E:226:LEU:HB2	2:F:62:LEU:CD1	2.34	0.58
1:A:132:GLU:OE2	1:A:143:LYS:HE2	2.04	0.57
1:C:145:LYS:CE	1:C:170:LYS:HB2	2.34	0.57
1:C:154:VAL:HG11	1:C:355:TYR:HB2	1.85	0.57
1:G:297:GLY:N	1:G:300:ASP:OD2	2.37	0.57
1:G:371:VAL:O	1:G:371:VAL:HG12	2.04	0.57
1:A:37:GLN:NE2	1:A:38:PRO:HD2	2.17	0.57
1:A:83:CYS:HA	1:A:140:GLN:HE22	1.70	0.57
1:E:290:VAL:HG22	1:E:291:PRO:CD	2.34	0.57
1:G:154:VAL:HG12	1:G:155:THR:N	2.19	0.57
1:G:286:LEU:HB3	1:G:292:VAL:HG21	1.85	0.57
1:C:330:ASN:CB	1:C:331:PRO:HD3	2.29	0.57
1:E:407:THR:O	1:E:429:PRO:HA	2.05	0.57
1:E:181:LEU:HD12	1:E:417:GLY:HA3	1.86	0.57
1:C:290:VAL:HG22	1:C:291:PRO:CD	2.34	0.57
1:C:65:LEU:HD21	1:C:158:VAL:HG12	1.87	0.57
1:G:101:MET:HB2	1:G:128:HIS:CG	2.40	0.57
1:G:200:SER:HB3	1:G:428:VAL:HG12	1.86	0.57
1:A:193:ASP:OD2	1:A:193:ASP:N	2.38	0.57
1:A:193:ASP:HB2	1:A:441:ASN:HD21	1.69	0.57
1:G:343:GLY:HA3	1:G:403:PHE:CD1	2.39	0.57
1:C:297:GLY:N	1:C:300:ASP:OD2	2.37	0.57
1:C:439:LEU:HG	1:C:450:ILE:CD1	2.34	0.57
1:A:226:LEU:HD12	1:A:226:LEU:O	2.03	0.57
1:A:24:PHE:CZ	1:A:233:CYS:HB2	2.40	0.57
1:A:36:SER:HB3	1:A:333:GLN:H	1.69	0.57
1:C:343:GLY:HA3	1:C:403:PHE:CE1	2.40	0.57
1:E:126:TYR:HD2	1:E:355:TYR:HE1	1.51	0.57
1:E:224:GLY:HA3	2:F:135:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:GLN:C	1:E:39:PHE:H	2.09	0.57
1:E:65:LEU:CD2	1:E:158:VAL:HG12	2.34	0.57
2:H:70:ASN:C	2:H:72:HIS:H	2.09	0.57
1:A:343:GLY:HA3	1:A:403:PHE:CD1	2.40	0.56
2:B:70:ASN:HB2	2:B:72:HIS:CE1	2.40	0.56
1:C:37:GLN:N	1:C:38:PRO:HD2	2.20	0.56
1:C:82:LEU:HD11	1:C:142:ILE:HG22	1.85	0.56
1:E:26:ARG:HG3	1:E:27:VAL:N	2.20	0.56
1:A:231:GLU:HG3	2:B:97:SER:OG	2.04	0.56
1:A:303:ASN:HD22	1:A:305:THR:HG22	1.70	0.56
1:A:407:THR:O	1:A:429:PRO:HA	2.05	0.56
1:A:65:LEU:CD2	1:A:158:VAL:HG12	2.35	0.56
1:G:97:LEU:HD22	1:G:133:LEU:HB3	1.87	0.56
1:E:269:GLN:O	1:E:273:VAL:HG23	2.04	0.56
1:C:145:LYS:HE2	1:C:168:ASP:OD1	2.05	0.56
1:E:360:ASP:OD2	1:E:362:LEU:HB3	2.05	0.56
2:F:111:SER:O	2:F:114:LEU:HB2	2.04	0.56
1:A:65:LEU:HD23	1:A:159:LEU:O	2.04	0.56
1:C:348:ASN:HB2	1:C:375:SER:HB2	1.86	0.56
1:E:36:SER:HB3	1:E:333:GLN:H	1.71	0.56
2:B:6:TYR:HA	2:B:9:ASN:HD22	1.71	0.56
1:C:37:GLN:O	1:C:39:PHE:N	2.38	0.56
1:E:243:LEU:N	1:E:243:LEU:HD23	2.20	0.56
1:E:313:PRO:HB2	1:G:273:VAL:HG22	1.88	0.56
1:G:348:ASN:CB	1:G:375:SER:HB2	2.35	0.56
2:H:12:GLU:O	2:H:17:GLN:HG3	2.06	0.56
1:C:37:GLN:C	1:C:39:PHE:H	2.09	0.56
2:D:111:SER:O	2:D:114:LEU:HB2	2.06	0.56
1:G:193:ASP:OD2	1:G:193:ASP:N	2.39	0.56
1:C:14:LEU:HD11	2:D:98:ILE:CG2	2.36	0.56
2:D:64:SER:OG	2:D:97:SER:HB2	2.06	0.56
2:F:67:LEU:HD23	2:F:76:LYS:HE3	1.86	0.56
1:A:348:ASN:HB2	1:A:375:SER:HB2	1.87	0.56
1:A:75:SER:O	1:A:77:VAL:HG23	2.06	0.56
1:C:393:PHE:N	1:C:393:PHE:CD2	2.72	0.56
2:D:45:VAL:HG23	2:D:46:GLU:N	2.21	0.56
2:F:66:SER:HB3	2:F:94:VAL:CG1	2.36	0.56
1:G:99:LYS:N	1:G:155:THR:HG23	2.16	0.56
1:G:407:THR:O	1:G:429:PRO:HA	2.06	0.56
1:A:77:VAL:CG1	1:A:79:VAL:HB	2.36	0.55
1:A:82:LEU:HD11	1:A:142:ILE:HG22	1.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:THR:HG23	1:C:408:PRO:HD2	1.87	0.55
1:A:145:LYS:CE	1:A:170:LYS:HB2	2.35	0.55
1:E:410:PHE:CE1	1:E:438:CYS:HB2	2.41	0.55
1:E:419:GLU:CD	1:E:419:GLU:N	2.59	0.55
1:G:132:GLU:OE2	1:G:143:LYS:HE2	2.06	0.55
1:A:306:LEU:O	1:A:306:LEU:HD12	2.06	0.55
2:B:6:TYR:CD1	2:B:40:MET:HG2	2.40	0.55
1:C:199:VAL:HG12	1:C:200:SER:N	2.22	0.55
1:C:348:ASN:CB	1:C:375:SER:HB2	2.36	0.55
1:A:193:ASP:C	1:A:194:ARG:HD3	2.26	0.55
1:A:26:ARG:HG3	1:A:27:VAL:N	2.21	0.55
1:C:26:ARG:HG3	1:C:27:VAL:H	1.71	0.55
2:F:58:HIS:CE1	2:F:107:MET:HB2	2.41	0.55
1:G:410:PHE:CE1	1:G:438:CYS:HB2	2.41	0.55
1:G:65:LEU:HD21	1:G:158:VAL:HG12	1.86	0.55
2:H:58:HIS:CE1	2:H:107:MET:HB2	2.41	0.55
1:A:306:LEU:O	1:A:308:GLN:N	2.38	0.55
1:C:99:LYS:N	1:C:155:THR:HG23	2.18	0.55
1:C:37:GLN:NE2	1:C:38:PRO:HD2	2.18	0.55
2:D:2:ALA:O	2:D:5:LEU:HB3	2.06	0.55
1:E:37:GLN:N	1:E:38:PRO:HD2	2.21	0.55
1:G:185:LYS:HE3	1:G:397:GLU:OE2	2.07	0.55
1:G:330:ASN:CB	1:G:331:PRO:HD3	2.32	0.55
1:A:68:ARG:HG3	1:A:179:ALA:HA	1.89	0.55
1:C:284:LEU:HD22	1:C:318:LEU:HB3	1.89	0.55
1:C:330:ASN:CB	1:C:331:PRO:CD	2.84	0.55
1:C:5:GLN:O	1:C:8:GLN:HB2	2.07	0.55
1:C:19:ALA:HB2	1:E:443:ARG:CZ	2.37	0.55
2:F:24:LYS:O	2:F:27:SER:HB3	2.06	0.55
1:C:14:LEU:HD11	2:D:98:ILE:HG22	1.89	0.55
1:A:274:GLU:O	1:A:277:LYS:HB3	2.07	0.55
1:A:37:GLN:N	1:A:38:PRO:HD2	2.21	0.55
1:C:99:LYS:HE2	1:C:150:VAL:HG12	1.89	0.55
1:C:154:VAL:HG12	1:C:155:THR:N	2.20	0.55
1:C:226:LEU:HB2	2:D:62:LEU:CD1	2.37	0.55
2:D:67:LEU:HD23	2:D:76:LYS:HE3	1.89	0.55
2:D:70:ASN:HB2	2:D:72:HIS:CE1	2.42	0.55
1:E:279:LEU:HD12	1:E:279:LEU:O	2.07	0.55
1:E:393:PHE:CD2	1:E:393:PHE:N	2.73	0.55
1:G:77:VAL:CG1	1:G:79:VAL:HB	2.36	0.55
1:G:451:SER:HB2	2:H:76:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:VAL:HG12	1:G:200:SER:N	2.22	0.55
1:E:13:LEU:HD13	2:F:38:LYS:HD2	1.89	0.54
1:E:5:GLN:O	1:E:8:GLN:HB2	2.07	0.54
1:C:21:ASN:H	1:E:237:HIS:CE1	2.24	0.54
1:C:343:GLY:HA3	1:C:403:PHE:CD1	2.42	0.54
1:C:360:ASP:OD2	1:C:362:LEU:HB3	2.07	0.54
2:D:6:TYR:HA	2:D:9:ASN:HD22	1.72	0.54
1:E:204:LEU:HD12	1:E:279:LEU:HB2	1.89	0.54
1:E:373:HIS:HA	1:E:393:PHE:O	2.07	0.54
1:E:77:VAL:CG1	1:E:79:VAL:HB	2.37	0.54
1:G:226:LEU:C	1:G:226:LEU:CD1	2.76	0.54
1:G:290:VAL:CG2	1:G:291:PRO:HD2	2.34	0.54
1:A:133:LEU:HD21	1:A:150:VAL:HG13	1.88	0.54
1:C:279:LEU:O	1:C:279:LEU:HD12	2.06	0.54
1:C:226:LEU:HD13	2:D:62:LEU:HD11	1.89	0.54
1:C:36:SER:HB3	1:C:333:GLN:H	1.72	0.54
1:E:228:ASP:OD1	1:E:229:GLU:N	2.39	0.54
1:E:303:ASN:HB2	1:E:305:THR:HG22	1.90	0.54
1:E:380:ASP:O	1:E:381:THR:HG23	2.08	0.54
1:E:68:ARG:O	1:E:72:HIS:HB2	2.07	0.54
1:G:68:ARG:O	1:G:72:HIS:HB2	2.07	0.54
1:A:145:LYS:HE2	1:A:168:ASP:OD1	2.07	0.54
1:A:68:ARG:O	1:A:72:HIS:HB2	2.07	0.54
2:B:58:HIS:CE1	2:B:107:MET:HB2	2.42	0.54
1:E:410:PHE:HA	1:E:429:PRO:HD3	1.90	0.54
1:G:279:LEU:O	1:G:279:LEU:HD12	2.08	0.54
1:G:303:ASN:HD22	1:G:305:THR:HG22	1.73	0.54
1:A:286:LEU:HB3	1:A:292:VAL:HG21	1.90	0.54
1:A:297:GLY:N	1:A:300:ASP:OD2	2.41	0.54
1:A:380:ASP:O	1:A:381:THR:HG23	2.07	0.54
1:A:65:LEU:HD21	1:A:158:VAL:C	2.27	0.54
1:E:290:VAL:CG2	1:E:291:PRO:HD2	2.37	0.54
1:E:371:VAL:HG12	1:E:371:VAL:O	2.07	0.54
1:A:154:VAL:HG12	1:A:155:THR:N	2.23	0.54
1:A:243:LEU:N	1:A:243:LEU:HD23	2.23	0.54
1:C:380:ASP:O	1:C:381:THR:HG23	2.06	0.54
1:E:407:THR:CG2	1:E:408:PRO:HD2	2.38	0.54
1:A:360:ASP:OD2	1:A:362:LEU:HB3	2.08	0.54
1:A:373:HIS:HA	1:A:393:PHE:O	2.07	0.54
1:C:303:ASN:HB2	1:C:305:THR:HG22	1.89	0.54
2:D:58:HIS:CE1	2:D:107:MET:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:PRO:O	1:E:423:VAL:HG22	2.06	0.54
1:G:82:LEU:HD13	1:G:93:VAL:HG11	1.89	0.54
2:H:6:TYR:CD1	2:H:40:MET:HG2	2.43	0.54
1:C:224:GLY:HA3	2:D:135:ILE:HG13	1.90	0.54
1:E:193:ASP:C	1:E:194:ARG:HD3	2.27	0.54
1:G:-2:HIS:O	1:G:-1:HIS:HB2	2.08	0.54
1:C:306:LEU:O	1:C:308:GLN:N	2.39	0.54
1:E:98:PHE:HA	1:E:155:THR:HG22	1.88	0.54
1:E:163:GLY:HA3	1:E:172:LEU:O	2.08	0.54
1:E:303:ASN:HA	1:G:303:ASN:HA	1.90	0.54
1:G:224:GLY:HA3	2:H:135:ILE:HG13	1.90	0.54
1:A:406:ASN:N	1:A:406:ASN:ND2	2.53	0.53
1:C:68:ARG:HG3	1:C:179:ALA:HA	1.90	0.53
1:C:26:ARG:NH1	1:C:289:SER:O	2.40	0.53
1:C:57:ARG:NH2	1:C:378:ALA:O	2.41	0.53
1:E:101:MET:HB2	1:E:128:HIS:CG	2.42	0.53
2:F:12:GLU:O	2:F:17:GLN:HG3	2.07	0.53
1:G:360:ASP:OD2	1:G:362:LEU:HB3	2.08	0.53
1:C:61:MET:HE3	1:C:158:VAL:HB	1.89	0.53
1:C:243:LEU:N	1:C:243:LEU:HD23	2.24	0.53
1:G:393:PHE:N	1:G:393:PHE:CD2	2.73	0.53
2:H:111:SER:O	2:H:114:LEU:HB2	2.08	0.53
1:A:419:GLU:CD	1:A:419:GLU:N	2.61	0.53
1:A:82:LEU:HD13	1:A:93:VAL:HG11	1.89	0.53
1:C:346:GLY:CA	1:C:405:GLY:HA3	2.39	0.53
1:E:407:THR:OG1	1:E:427:THR:HB	2.07	0.53
1:G:65:LEU:HD21	1:G:158:VAL:C	2.29	0.53
1:G:307:PRO:HG3	1:G:393:PHE:CZ	2.43	0.53
1:A:303:ASN:ND2	1:A:308:GLN:HA	2.22	0.53
1:C:26:ARG:CG	1:C:27:VAL:N	2.72	0.53
1:C:98:PHE:HA	1:C:155:THR:HG22	1.91	0.53
1:E:83:CYS:HA	1:E:140:GLN:HE22	1.72	0.53
1:G:29:VAL:HG11	1:G:291:PRO:CG	2.18	0.53
2:H:45:VAL:HG23	2:H:46:GLU:N	2.22	0.53
1:C:163:GLY:HA3	1:C:172:LEU:O	2.08	0.53
1:C:266:LYS:HG3	1:C:267:LYS:HG3	1.91	0.53
1:C:77:VAL:CG1	1:C:79:VAL:HB	2.38	0.53
2:F:6:TYR:HA	2:F:9:ASN:HD22	1.74	0.53
1:G:83:CYS:HA	1:G:140:GLN:HE22	1.73	0.53
1:G:99:LYS:HE2	1:G:150:VAL:HG12	1.90	0.53
2:H:52:ASN:CB	2:H:55:ALA:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:NH2	1:A:378:ALA:O	2.42	0.53
1:C:290:VAL:CG2	1:C:291:PRO:HD2	2.38	0.53
1:C:371:VAL:O	1:C:371:VAL:HG12	2.08	0.53
1:C:83:CYS:HA	1:C:140:GLN:HE22	1.73	0.53
1:E:226:LEU:C	1:E:226:LEU:CD1	2.76	0.53
2:F:23:TYR:CD1	2:F:38:LYS:HE2	2.44	0.53
1:A:212:LEU:O	1:A:215:THR:N	2.42	0.53
1:E:65:LEU:HD21	1:E:158:VAL:HG12	1.90	0.53
2:F:2:ALA:O	2:F:5:LEU:HB3	2.09	0.53
1:A:438:CYS:SG	1:A:439:LEU:N	2.82	0.53
1:C:439:LEU:HD12	1:C:450:ILE:HD11	1.91	0.53
1:G:330:ASN:CB	1:G:331:PRO:CD	2.87	0.53
2:H:125:ASN:C	2:H:127:GLN:N	2.62	0.53
1:A:351:ASP:HA	1:A:354:ARG:HD2	1.90	0.53
2:B:52:ASN:CB	2:B:55:ALA:HB2	2.39	0.53
1:C:75:SER:O	1:C:77:VAL:HG23	2.09	0.53
1:E:193:ASP:CB	1:E:441:ASN:ND2	2.67	0.53
1:A:199:VAL:HG12	1:A:200:SER:N	2.23	0.52
1:A:266:LYS:HG3	1:A:267:LYS:HG3	1.91	0.52
1:A:279:LEU:HD12	1:A:279:LEU:O	2.08	0.52
1:E:197:LEU:HD21	1:E:218:LEU:HD11	1.90	0.52
1:E:212:LEU:O	1:E:215:THR:N	2.42	0.52
1:E:269:GLN:NE2	1:G:320:THR:HB	2.24	0.52
2:H:66:SER:HB3	2:H:94:VAL:CG1	2.40	0.52
1:A:99:LYS:N	1:A:155:THR:HG23	2.17	0.52
1:A:303:ASN:HB2	1:A:305:THR:HG22	1.91	0.52
2:B:23:TYR:CD2	2:B:24:LYS:N	2.77	0.52
1:A:193:ASP:CB	1:A:441:ASN:ND2	2.69	0.52
1:C:419:GLU:N	1:C:419:GLU:CD	2.63	0.52
1:C:200:SER:HB3	1:C:428:VAL:HG12	1.92	0.52
1:E:297:GLY:N	1:E:300:ASP:OD2	2.43	0.52
1:E:439:LEU:HD12	1:E:450:ILE:HD11	1.89	0.52
1:E:98:PHE:HA	1:E:155:THR:CG2	2.39	0.52
2:D:12:GLU:O	2:D:17:GLN:HG3	2.10	0.52
1:G:37:GLN:N	1:G:38:PRO:HD2	2.24	0.52
1:E:303:ASN:ND2	1:E:308:GLN:HA	2.24	0.52
1:E:315:MET:HG2	1:G:314:CYS:SG	2.49	0.52
2:F:10:ILE:O	2:F:14:VAL:HG23	2.10	0.52
1:G:303:ASN:HB2	1:G:305:THR:HG22	1.90	0.52
1:G:407:THR:OG1	1:G:427:THR:HB	2.09	0.52
1:G:58:LEU:HD21	1:G:95:GLY:CA	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LEU:O	2:B:125:ASN:N	2.38	0.52
1:C:274:GLU:O	1:C:277:LYS:HB3	2.09	0.52
1:C:82:LEU:HD13	1:C:93:VAL:HG11	1.91	0.52
1:E:148:ILE:HA	1:E:176:TYR:CE2	2.42	0.52
1:E:395:PHE:H	1:E:395:PHE:HD1	1.58	0.52
1:G:395:PHE:HD1	1:G:395:PHE:H	1.58	0.52
1:A:212:LEU:O	1:A:213:LEU:C	2.46	0.52
1:A:371:VAL:O	1:A:371:VAL:HG12	2.09	0.52
1:C:193:ASP:C	1:C:194:ARG:HD3	2.30	0.52
1:C:68:ARG:O	1:C:72:HIS:HB2	2.09	0.52
1:E:348:ASN:CB	1:E:375:SER:HB2	2.40	0.52
2:F:41:LEU:HD22	2:F:103:ILE:HD12	1.90	0.52
1:G:21:ASN:OD1	2:H:36:GLN:HB2	2.10	0.52
1:A:200:SER:HB3	1:A:428:VAL:HG12	1.91	0.52
1:A:14:LEU:HD11	2:B:98:ILE:HG22	1.92	0.52
1:C:225:GLN:HE21	2:D:133:SER:HB2	1.74	0.52
1:E:99:LYS:N	1:E:155:THR:HG23	2.17	0.52
1:A:26:ARG:HD3	1:A:290:VAL:HG23	1.91	0.52
1:A:459:ASP:C	1:A:461:ASP:H	2.11	0.52
1:C:82:LEU:HB2	1:C:137:ASP:HB2	1.92	0.52
1:C:264:LEU:HD23	1:C:265:THR:N	2.25	0.52
1:C:303:ASN:ND2	1:C:308:GLN:HA	2.24	0.52
1:C:393:PHE:HD2	1:C:393:PHE:N	2.08	0.52
1:E:330:ASN:CB	1:E:331:PRO:HD3	2.33	0.52
1:E:393:PHE:HD2	1:E:393:PHE:N	2.08	0.52
1:G:98:PHE:HA	1:G:155:THR:HG22	1.91	0.52
1:G:197:LEU:HD21	1:G:218:LEU:HD11	1.92	0.52
1:A:393:PHE:CD2	1:A:393:PHE:N	2.75	0.51
2:B:68:ILE:CD1	2:B:68:ILE:N	2.72	0.51
2:D:10:ILE:O	2:D:14:VAL:HG23	2.10	0.51
1:E:199:VAL:HG12	1:E:200:SER:N	2.24	0.51
1:E:330:ASN:CB	1:E:331:PRO:CD	2.87	0.51
1:E:351:ASP:O	1:E:352:ILE:C	2.49	0.51
2:F:68:ILE:N	2:F:68:ILE:CD1	2.73	0.51
2:H:6:TYR:HA	2:H:9:ASN:HD22	1.75	0.51
1:E:197:LEU:HB3	1:E:241:VAL:HG22	1.91	0.51
2:H:62:LEU:HD23	2:H:62:LEU:C	2.30	0.51
1:C:65:LEU:HD21	1:C:158:VAL:C	2.31	0.51
2:D:86:GLU:OE2	2:D:86:GLU:HA	2.10	0.51
1:G:348:ASN:HB3	1:G:375:SER:HB2	1.92	0.51
1:A:14:LEU:HD11	2:B:98:ILE:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:HD22	2:B:103:ILE:HD12	1.92	0.51
1:E:61:MET:HE3	1:E:158:VAL:HB	1.92	0.51
2:F:122:LEU:O	2:F:125:ASN:N	2.42	0.51
2:H:10:ILE:O	2:H:14:VAL:HG23	2.10	0.51
1:C:5:GLN:HG3	1:C:193:ASP:OD1	2.11	0.51
1:E:154:VAL:HG12	1:E:155:THR:N	2.26	0.51
1:A:65:LEU:HD21	1:A:158:VAL:HG12	1.93	0.51
1:G:226:LEU:HD12	1:G:226:LEU:O	2.10	0.51
1:G:57:ARG:NH2	1:G:378:ALA:O	2.44	0.51
1:A:5:GLN:HG3	1:A:193:ASP:OD1	2.10	0.51
1:C:65:LEU:HD23	1:C:159:LEU:O	2.10	0.51
1:C:239:SER:O	1:C:240:ARG:HG2	2.10	0.51
1:C:303:ASN:HD22	1:C:305:THR:HG22	1.74	0.51
2:D:6:TYR:CD1	2:D:40:MET:HG2	2.46	0.51
1:G:204:LEU:HD12	1:G:279:LEU:HB2	1.93	0.51
1:G:212:LEU:O	1:G:215:THR:N	2.44	0.51
1:G:351:ASP:HA	1:G:354:ARG:HD2	1.93	0.51
1:A:264:LEU:HD23	1:A:265:THR:N	2.25	0.51
1:A:225:GLN:NE2	2:B:133:SER:HB2	2.26	0.51
2:B:64:SER:OG	2:B:97:SER:HB2	2.11	0.51
2:B:81:ARG:NH1	2:B:108:LEU:O	2.44	0.51
1:C:53:ILE:HG22	1:C:55:ALA:H	1.76	0.51
1:C:216:GLN:HE21	2:D:115:PHE:HD1	1.57	0.51
1:G:345:SER:C	1:G:405:GLY:HA3	2.31	0.51
1:A:224:GLY:HA3	2:B:135:ILE:HG13	1.93	0.51
1:E:264:LEU:HD23	1:E:265:THR:N	2.26	0.51
1:E:82:LEU:HD13	1:E:93:VAL:HG11	1.91	0.51
1:G:231:GLU:HG3	2:H:97:SER:OG	2.11	0.51
1:C:410:PHE:HA	1:C:429:PRO:HD3	1.93	0.51
1:E:439:LEU:CG	1:E:450:ILE:HD11	2.41	0.51
1:E:99:LYS:HE2	1:E:150:VAL:HG12	1.93	0.51
2:F:42:TYR:O	2:F:45:VAL:HG22	2.11	0.51
1:G:239:SER:O	1:G:240:ARG:HG2	2.10	0.51
1:G:284:LEU:HD22	1:G:318:LEU:HB3	1.92	0.51
1:G:36:SER:HB3	1:G:333:GLN:H	1.76	0.51
1:G:5:GLN:O	1:G:8:GLN:HB2	2.10	0.51
1:C:19:ALA:HB1	1:E:193:ASP:OD2	2.11	0.50
1:E:65:LEU:HD21	1:E:158:VAL:C	2.32	0.50
1:E:307:PRO:HG3	1:E:393:PHE:CZ	2.46	0.50
1:E:351:ASP:HA	1:E:354:ARG:HD2	1.93	0.50
1:A:225:GLN:HE21	2:B:133:SER:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:TYR:CD1	2:B:38:LYS:HE2	2.46	0.50
1:A:13:LEU:HD13	2:B:38:LYS:HD2	1.92	0.50
1:C:410:PHE:CE1	1:C:438:CYS:HB2	2.45	0.50
2:D:41:LEU:HD22	2:D:103:ILE:HD12	1.92	0.50
1:E:200:SER:HB3	1:E:428:VAL:HG12	1.92	0.50
1:G:5:GLN:HG3	1:G:193:ASP:OD1	2.11	0.50
2:H:2:ALA:O	2:H:5:LEU:HB3	2.12	0.50
1:A:211:SER:HA	1:A:435:GLN:NE2	2.27	0.50
1:E:225:GLN:NE2	2:F:133:SER:HB2	2.26	0.50
2:H:23:TYR:CD2	2:H:24:LYS:N	2.79	0.50
2:H:24:LYS:O	2:H:27:SER:HB3	2.10	0.50
1:C:423:VAL:HG12	1:C:425:LEU:HD23	1.93	0.50
1:E:154:VAL:HG11	1:E:355:TYR:CB	2.41	0.50
1:G:393:PHE:N	1:G:393:PHE:HD2	2.10	0.50
2:B:2:ALA:O	2:B:5:LEU:HB3	2.12	0.50
1:C:373:HIS:HA	1:C:393:PHE:O	2.11	0.50
1:C:231:GLU:CG	2:D:97:SER:OG	2.60	0.50
1:C:29:VAL:HG11	1:C:291:PRO:CG	2.13	0.50
1:C:315:MET:C	1:C:317:PRO:HD3	2.33	0.50
1:E:132:GLU:OE2	1:E:143:LYS:HE2	2.12	0.50
2:F:52:ASN:CB	2:F:55:ALA:HB2	2.42	0.50
1:G:351:ASP:O	1:G:352:ILE:C	2.50	0.50
1:A:26:ARG:CD	1:A:290:VAL:HG23	2.42	0.50
2:B:72:HIS:HD2	2:B:72:HIS:O	1.94	0.50
1:C:65:LEU:HD12	1:C:179:ALA:HB2	1.94	0.50
1:G:266:LYS:HG3	1:G:267:LYS:HG3	1.94	0.50
1:G:306:LEU:HD12	1:G:306:LEU:O	2.11	0.50
1:A:330:ASN:CB	1:A:331:PRO:CD	2.89	0.50
1:E:266:LYS:HG3	1:E:267:LYS:HG3	1.94	0.50
1:E:439:LEU:HG	1:E:450:ILE:HD11	1.94	0.50
1:G:419:GLU:N	1:G:419:GLU:CD	2.64	0.50
1:A:459:ASP:O	1:A:462:LEU:HG	2.13	0.49
2:B:99:HIS:ND1	2:B:100:VAL:O	2.40	0.49
2:D:125:ASN:C	2:D:127:GLN:N	2.64	0.49
1:E:212:LEU:O	1:E:213:LEU:C	2.48	0.49
1:E:26:ARG:HD3	1:E:290:VAL:HG23	1.94	0.49
1:G:172:LEU:HD22	3:G:474:HOH:O	2.11	0.49
2:B:86:GLU:HA	2:B:86:GLU:OE2	2.11	0.49
1:C:151:SER:O	1:C:357:SER:N	2.45	0.49
1:C:225:GLN:NE2	2:D:133:SER:HB2	2.27	0.49
1:E:221:VAL:HG21	1:E:452:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:VAL:HG11	1:G:355:TYR:CB	2.41	0.49
1:A:190:LEU:HB2	1:A:443:ARG:HB2	1.94	0.49
1:A:303:ASN:HD21	1:A:308:GLN:HA	1.77	0.49
1:A:307:PRO:HG3	1:A:393:PHE:CZ	2.47	0.49
1:A:410:PHE:HA	1:A:429:PRO:HD3	1.94	0.49
1:A:98:PHE:HA	1:A:155:THR:HG22	1.93	0.49
2:B:52:ASN:HB3	2:B:55:ALA:HB2	1.95	0.49
1:C:399:PRO:O	1:C:423:VAL:HG22	2.12	0.49
1:E:303:ASN:HB3	1:G:304:TYR:CD1	2.47	0.49
2:F:32:VAL:HG11	2:F:40:MET:HE1	1.94	0.49
1:G:67:ASN:O	1:G:71:GLN:HG2	2.12	0.49
1:A:410:PHE:CE1	1:A:438:CYS:HB2	2.44	0.49
1:C:226:LEU:C	1:C:226:LEU:CD1	2.81	0.49
2:F:45:VAL:HG23	2:F:46:GLU:N	2.27	0.49
1:G:218:LEU:HD22	1:G:431:PHE:CE2	2.48	0.49
2:D:66:SER:HB3	2:D:94:VAL:CG1	2.42	0.49
2:D:81:ARG:NH1	2:D:108:LEU:O	2.45	0.49
1:E:11:HIS:N	1:E:11:HIS:CD2	2.81	0.49
1:E:275:ALA:O	1:E:276:VAL:C	2.51	0.49
1:E:14:LEU:HD11	2:F:98:ILE:CG2	2.42	0.49
2:B:103:ILE:N	2:B:104:GLN:HE21	2.10	0.49
2:B:62:LEU:C	2:B:62:LEU:HD23	2.33	0.49
1:C:157:THR:HG23	1:C:371:VAL:HG11	1.93	0.49
1:C:67:ASN:O	1:C:71:GLN:HG2	2.12	0.49
1:E:159:LEU:N	1:E:159:LEU:HD23	2.25	0.49
1:C:185:LYS:HE3	1:C:397:GLU:OE2	2.12	0.49
1:E:5:GLN:HG3	1:E:193:ASP:OD1	2.12	0.49
1:E:345:SER:C	1:E:405:GLY:HA3	2.33	0.49
1:G:439:LEU:HD12	1:G:450:ILE:HD11	1.94	0.49
1:A:348:ASN:HB3	1:A:375:SER:HB2	1.95	0.49
1:A:395:PHE:H	1:A:395:PHE:HD1	1.58	0.49
2:B:125:ASN:C	2:B:127:GLN:N	2.66	0.49
1:C:351:ASP:O	1:C:352:ILE:C	2.50	0.49
1:C:407:THR:CG2	1:C:408:PRO:HD2	2.41	0.49
2:D:62:LEU:C	2:D:62:LEU:HD23	2.33	0.49
1:E:60:GLN:O	1:E:63:PRO:HD2	2.13	0.49
2:F:81:ARG:NH1	2:F:108:LEU:O	2.46	0.49
1:G:82:LEU:HB2	1:G:137:ASP:HB2	1.95	0.49
1:G:264:LEU:HD23	1:G:265:THR:N	2.27	0.49
1:G:98:PHE:HA	1:G:155:THR:CG2	2.43	0.49
1:A:26:ARG:NH1	1:A:289:SER:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASP:O	1:C:363:GLU:HB3	2.13	0.49
1:E:151:SER:O	1:E:357:SER:N	2.46	0.49
1:G:75:SER:O	1:G:77:VAL:HG23	2.13	0.49
1:A:204:LEU:HD12	1:A:279:LEU:HB2	1.94	0.49
1:A:26:ARG:HG3	1:A:27:VAL:H	1.77	0.49
1:A:444:SER:O	1:A:445:LEU:HB2	2.12	0.49
1:C:351:ASP:HA	1:C:354:ARG:HD2	1.94	0.49
1:C:218:LEU:HD22	1:C:431:PHE:CE2	2.47	0.49
1:C:237:HIS:CE1	1:E:21:ASN:H	2.31	0.49
1:E:185:LYS:HE3	1:E:397:GLU:OE2	2.12	0.49
1:A:346:GLY:CA	1:A:405:GLY:HA3	2.43	0.48
2:B:10:ILE:O	2:B:14:VAL:HG23	2.13	0.48
2:D:45:VAL:CG2	2:D:46:GLU:N	2.76	0.48
1:A:221:VAL:HG21	1:A:452:PHE:HE2	1.78	0.48
1:A:3:SER:OG	2:B:75:HIS:ND1	2.34	0.48
1:E:406:ASN:ND2	1:E:406:ASN:N	2.47	0.48
1:G:95:GLY:CA	1:G:135:LEU:HD11	2.42	0.48
1:G:275:ALA:O	1:G:276:VAL:C	2.51	0.48
1:G:423:VAL:HG12	1:G:425:LEU:HD23	1.96	0.48
2:H:64:SER:OG	2:H:97:SER:HB2	2.12	0.48
1:A:2:PHE:CG	1:A:439:LEU:HD12	2.48	0.48
1:A:7:ALA:O	1:A:9:ARG:N	2.47	0.48
1:E:57:ARG:NH2	1:E:378:ALA:O	2.47	0.48
1:G:148:ILE:HA	1:G:176:TYR:CE2	2.46	0.48
1:G:410:PHE:HA	1:G:429:PRO:HD3	1.94	0.48
1:A:11:HIS:CD2	1:A:11:HIS:N	2.81	0.48
1:C:98:PHE:HA	1:C:155:THR:CG2	2.43	0.48
1:C:182:ALA:HB1	1:C:183:PRO:CD	2.37	0.48
1:C:373:HIS:O	1:C:376:PRO:HD3	2.13	0.48
2:D:24:LYS:O	2:D:27:SER:HB3	2.13	0.48
1:E:452:PHE:N	1:E:452:PHE:CD1	2.81	0.48
2:H:41:LEU:HD22	2:H:103:ILE:HD12	1.94	0.48
1:A:351:ASP:O	1:A:352:ILE:C	2.51	0.48
2:B:32:VAL:HG11	2:B:40:MET:HE1	1.95	0.48
2:B:45:VAL:HG23	2:B:46:GLU:N	2.27	0.48
1:E:430:ASP:OD1	1:E:432:SER:HB3	2.13	0.48
1:G:24:PHE:CZ	1:G:233:CYS:HB2	2.49	0.48
1:G:319:ALA:CB	1:G:325:LEU:HD22	2.42	0.48
1:A:269:GLN:NE2	1:C:320:THR:HB	2.29	0.48
1:A:67:ASN:O	1:A:71:GLN:HG2	2.14	0.48
1:C:443:ARG:CZ	1:E:19:ALA:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:ALA:O	1:E:321:ALA:N	2.47	0.48
1:E:37:GLN:H	1:E:37:GLN:CD	2.17	0.48
1:E:94:VAL:HB	3:E:484:HOH:O	2.12	0.48
1:G:60:GLN:O	1:G:63:PRO:HD2	2.14	0.48
2:B:24:LYS:O	2:B:27:SER:HB3	2.12	0.48
1:G:348:ASN:HB2	1:G:375:SER:HB2	1.95	0.48
2:H:42:TYR:O	2:H:45:VAL:HG22	2.13	0.48
2:H:68:ILE:CD1	2:H:68:ILE:N	2.77	0.48
1:G:14:LEU:HD11	2:H:98:ILE:CG2	2.44	0.48
1:A:37:GLN:CD	1:A:37:GLN:H	2.17	0.48
2:B:23:TYR:CG	2:B:24:LYS:N	2.82	0.48
2:B:42:TYR:O	2:B:45:VAL:HG22	2.14	0.48
1:E:419:GLU:O	1:E:420:ASP:C	2.52	0.48
1:G:11:HIS:N	1:G:11:HIS:CD2	2.80	0.48
1:G:162:PHE:HB3	1:G:175:ASP:O	2.14	0.48
1:G:151:SER:O	1:G:357:SER:N	2.45	0.48
1:C:21:ASN:OD1	2:D:36:GLN:HB2	2.14	0.48
1:E:244:ALA:HA	1:E:295:MET:HB2	1.96	0.48
1:E:218:LEU:HD22	1:E:431:PHE:CE2	2.49	0.48
1:E:225:GLN:HE21	2:F:133:SER:HB2	1.78	0.48
1:G:311:LEU:HA	1:G:311:LEU:HD23	1.63	0.48
1:G:419:GLU:O	1:G:420:ASP:C	2.52	0.48
1:A:163:GLY:HA3	1:A:172:LEU:O	2.13	0.48
1:A:284:LEU:HD22	1:A:318:LEU:HB3	1.96	0.48
2:D:52:ASN:HB3	2:D:55:ALA:HB2	1.96	0.48
1:E:82:LEU:HB2	1:E:137:ASP:HB2	1.96	0.48
1:E:157:THR:HG23	1:E:371:VAL:HG11	1.95	0.48
1:A:378:ALA:HA	1:A:379:PRO:HD3	1.75	0.47
1:A:97:LEU:CD2	1:A:133:LEU:HB3	2.44	0.47
1:E:136:GLU:HG2	1:E:141:ARG:HB3	1.96	0.47
1:E:29:VAL:HG11	1:E:291:PRO:CG	2.16	0.47
1:E:319:ALA:CB	1:E:325:LEU:HD22	2.44	0.47
1:G:163:GLY:HA3	1:G:172:LEU:O	2.14	0.47
1:G:193:ASP:CB	1:G:443:ARG:NH1	2.64	0.47
2:H:103:ILE:N	2:H:104:GLN:HE21	2.12	0.47
1:A:151:SER:O	1:A:357:SER:N	2.47	0.47
1:C:204:LEU:HD12	1:C:279:LEU:HB2	1.96	0.47
1:C:307:PRO:HG3	1:C:393:PHE:CZ	2.48	0.47
2:D:52:ASN:CB	2:D:55:ALA:HB2	2.43	0.47
1:E:355:TYR:N	1:E:355:TYR:CD1	2.82	0.47
1:E:198:LEU:HB3	1:E:428:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:GLN:HE21	2:F:115:PHE:HD1	1.61	0.47
1:G:373:HIS:HA	1:G:393:PHE:O	2.14	0.47
1:A:83:CYS:HA	1:A:140:GLN:NE2	2.28	0.47
2:B:72:HIS:O	2:B:72:HIS:CD2	2.68	0.47
1:C:228:ASP:OD1	1:C:229:GLU:N	2.45	0.47
1:C:195:PHE:HB2	1:C:238:VAL:HG22	1.96	0.47
1:C:86:GLN:O	1:C:87:PRO:C	2.53	0.47
1:E:97:LEU:CD2	1:E:133:LEU:HB3	2.43	0.47
1:G:65:LEU:HD12	1:G:179:ALA:HB2	1.95	0.47
1:G:37:GLN:H	1:G:37:GLN:CD	2.18	0.47
1:A:416:ARG:HA	1:A:421:GLN:O	2.14	0.47
1:C:19:ALA:CB	1:E:193:ASP:OD2	2.63	0.47
1:G:145:LYS:HE2	1:G:168:ASP:OD1	2.15	0.47
1:G:315:MET:C	1:G:317:PRO:HD3	2.33	0.47
1:G:157:THR:HG23	1:G:371:VAL:HG11	1.96	0.47
1:C:37:GLN:CD	1:C:37:GLN:H	2.17	0.47
2:D:23:TYR:CD1	2:D:38:LYS:HE2	2.50	0.47
2:D:72:HIS:O	2:D:72:HIS:HD2	1.97	0.47
1:E:99:LYS:HE2	1:E:150:VAL:CG1	2.44	0.47
1:E:153:LEU:HD12	1:E:153:LEU:N	2.30	0.47
1:E:398:CYS:SG	1:E:423:VAL:HG21	2.54	0.47
2:F:125:ASN:C	2:F:127:GLN:N	2.67	0.47
2:F:62:LEU:C	2:F:62:LEU:HD23	2.33	0.47
1:G:136:GLU:HG2	1:G:141:ARG:HB3	1.96	0.47
1:G:239:SER:O	1:G:240:ARG:CG	2.62	0.47
1:C:-2:HIS:O	1:C:-1:HIS:HB2	2.15	0.47
1:C:395:PHE:HD1	1:C:395:PHE:H	1.57	0.47
2:D:122:LEU:O	2:D:125:ASN:N	2.46	0.47
1:E:423:VAL:HG12	1:E:425:LEU:HD23	1.97	0.47
1:E:439:LEU:HG	1:E:450:ILE:CD1	2.44	0.47
1:G:228:ASP:OD1	1:G:229:GLU:N	2.43	0.47
1:G:221:VAL:HG21	1:G:452:PHE:HE2	1.80	0.47
1:C:65:LEU:HD22	1:C:158:VAL:HG12	1.96	0.47
2:D:68:ILE:N	2:D:68:ILE:CD1	2.77	0.47
1:E:65:LEU:HD23	1:E:159:LEU:C	2.34	0.47
1:E:306:LEU:HD12	1:E:306:LEU:O	2.14	0.47
1:E:37:GLN:HB2	1:E:38:PRO:CD	2.45	0.47
1:A:226:LEU:HB3	2:B:23:TYR:OH	2.15	0.47
2:B:59:VAL:HG12	2:B:60:THR:N	2.29	0.47
1:C:212:LEU:O	1:C:215:THR:N	2.48	0.47
1:A:303:ASN:HB3	1:C:304:TYR:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:TYR:CD2	2:D:24:LYS:N	2.81	0.47
2:D:70:ASN:O	2:D:72:HIS:N	2.46	0.47
1:E:303:ASN:HD21	1:E:308:GLN:HA	1.80	0.47
1:E:416:ARG:HA	1:E:421:GLN:O	2.15	0.47
1:G:346:GLY:CA	1:G:405:GLY:HA3	2.45	0.47
1:A:393:PHE:HD2	1:A:393:PHE:N	2.13	0.47
1:A:65:LEU:HD12	1:A:179:ALA:HB2	1.97	0.47
1:A:82:LEU:HB2	1:A:137:ASP:HB2	1.96	0.47
1:A:86:GLN:O	1:A:87:PRO:C	2.53	0.47
1:C:83:CYS:HA	1:C:140:GLN:NE2	2.30	0.47
1:E:395:PHE:N	1:E:395:PHE:CD1	2.82	0.47
1:A:26:ARG:CG	1:A:27:VAL:N	2.77	0.47
1:A:315:MET:C	1:A:317:PRO:HD3	2.35	0.47
1:A:418:PRO:CB	1:A:419:GLU:OE1	2.62	0.47
1:A:423:VAL:HG12	1:A:425:LEU:HD23	1.97	0.47
1:C:11:HIS:CD2	1:C:11:HIS:N	2.82	0.47
1:E:145:LYS:HE2	1:E:168:ASP:OD1	2.15	0.47
1:E:348:ASN:HB2	1:E:375:SER:HB2	1.97	0.47
2:F:38:LYS:HD3	2:F:99:HIS:CE1	2.50	0.47
1:G:193:ASP:C	1:G:194:ARG:HD3	2.35	0.47
1:G:198:LEU:HB3	1:G:428:VAL:HG21	1.97	0.47
1:G:86:GLN:NE2	1:G:86:GLN:HA	2.29	0.47
1:A:78:GLY:O	1:A:91:CYS:HB2	2.15	0.46
1:C:419:GLU:O	1:C:420:ASP:C	2.53	0.46
1:C:211:SER:HA	1:C:435:GLN:NE2	2.30	0.46
1:C:438:CYS:SG	1:C:439:LEU:N	2.88	0.46
1:G:226:LEU:HD13	2:H:62:LEU:HD11	1.96	0.46
2:H:52:ASN:HB3	2:H:55:ALA:HB2	1.95	0.46
1:A:153:LEU:HD12	1:A:153:LEU:N	2.30	0.46
1:A:65:LEU:HD23	1:A:159:LEU:C	2.36	0.46
2:F:23:TYR:CD2	2:F:24:LYS:N	2.81	0.46
1:A:395:PHE:CD1	1:A:395:PHE:N	2.83	0.46
1:A:73:TRP:HZ3	1:A:92:CYS:SG	2.38	0.46
1:C:95:GLY:CA	1:C:135:LEU:HD11	2.41	0.46
1:C:145:LYS:NZ	1:C:168:ASP:HB2	2.30	0.46
1:C:428:VAL:HA	1:C:429:PRO:HD2	1.72	0.46
1:E:226:LEU:O	1:E:226:LEU:HD12	2.14	0.46
1:G:65:LEU:HD22	1:G:158:VAL:HG12	1.98	0.46
1:A:98:PHE:HA	1:A:155:THR:CG2	2.45	0.46
1:A:208:GLY:N	3:A:474:HOH:O	2.48	0.46
1:A:216:GLN:HE21	2:B:115:PHE:HD1	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ASP:OD1	1:A:432:SER:HB3	2.15	0.46
2:D:23:TYR:CG	2:D:24:LYS:N	2.84	0.46
1:E:315:MET:C	1:E:317:PRO:HD3	2.35	0.46
2:F:59:VAL:HG12	2:F:60:THR:N	2.30	0.46
1:A:182:ALA:HB1	1:A:183:PRO:CD	2.39	0.46
2:B:116:ASN:N	2:B:116:ASN:ND2	2.44	0.46
1:C:197:LEU:HD21	1:C:218:LEU:HD11	1.97	0.46
1:C:378:ALA:HA	1:C:379:PRO:HD3	1.75	0.46
1:C:410:PHE:CD2	1:C:449:PRO:HG3	2.51	0.46
1:E:67:ASN:O	1:E:71:GLN:HG2	2.16	0.46
1:E:78:GLY:O	1:E:91:CYS:HB2	2.16	0.46
2:F:23:TYR:CE1	2:F:38:LYS:HE2	2.50	0.46
1:A:369:LEU:CD2	1:A:423:VAL:HG11	2.46	0.46
1:E:83:CYS:HA	1:E:140:GLN:NE2	2.31	0.46
1:E:360:ASP:O	1:E:363:GLU:HB3	2.16	0.46
2:F:103:ILE:N	2:F:104:GLN:HE21	2.14	0.46
1:G:145:LYS:NZ	1:G:168:ASP:HB2	2.30	0.46
1:G:333:GLN:HG3	1:G:342:LEU:HD13	1.95	0.46
1:G:399:PRO:O	1:G:423:VAL:HG22	2.15	0.46
1:G:86:GLN:O	1:G:87:PRO:C	2.54	0.46
1:G:97:LEU:HG	1:G:159:LEU:CD2	2.45	0.46
1:C:-1:HIS:ND1	1:C:0:GLY:N	2.63	0.46
1:E:306:LEU:HD23	1:E:393:PHE:HE1	1.79	0.46
2:F:52:ASN:HB3	2:F:55:ALA:HB2	1.97	0.46
1:G:26:ARG:HD3	1:G:290:VAL:HG23	1.97	0.46
1:G:99:LYS:HE2	1:G:150:VAL:CG1	2.45	0.46
2:H:23:TYR:CD1	2:H:38:LYS:HE2	2.50	0.46
1:A:228:ASP:OD1	1:A:229:GLU:N	2.47	0.46
2:D:115:PHE:O	2:D:116:ASN:C	2.55	0.46
2:D:59:VAL:O	2:D:82:GLU:HB2	2.15	0.46
1:G:277:LYS:HE2	1:G:281:GLU:CD	2.36	0.46
1:G:452:PHE:N	1:G:452:PHE:CD1	2.84	0.46
2:H:23:TYR:CG	2:H:24:LYS:N	2.83	0.46
2:H:85:LEU:C	2:H:85:LEU:HD12	2.36	0.46
1:A:373:HIS:O	1:A:376:PRO:HD3	2.16	0.46
1:C:97:LEU:CD2	1:C:133:LEU:HB3	2.43	0.46
1:C:440:VAL:HG22	1:C:447:CYS:SG	2.56	0.46
1:C:60:GLN:O	1:C:63:PRO:HD2	2.16	0.46
1:E:333:GLN:HG3	1:E:342:LEU:HD13	1.98	0.46
2:F:99:HIS:ND1	2:F:100:VAL:O	2.45	0.46
2:F:23:TYR:CD1	2:F:34:VAL:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:GLU:HA	2:F:86:GLU:OE2	2.15	0.46
2:H:23:TYR:CD1	2:H:34:VAL:HG22	2.50	0.46
1:A:372:ARG:NH1	1:A:395:PHE:O	2.49	0.46
1:C:60:GLN:OE1	1:C:390:THR:HG23	2.16	0.46
1:E:194:ARG:HG3	1:E:194:ARG:NH1	2.31	0.46
1:G:216:GLN:HE21	2:H:115:PHE:HD1	1.63	0.46
2:H:45:VAL:CG2	2:H:46:GLU:N	2.79	0.46
1:A:198:LEU:HB3	1:A:428:VAL:HG21	1.97	0.45
1:A:80:LYS:HD3	1:A:84:GLU:HB2	1.98	0.45
2:B:3:ASP:CG	2:B:4:GLN:N	2.69	0.45
1:C:239:SER:O	1:C:240:ARG:CG	2.64	0.45
1:E:180:ASP:HA	1:E:370:ARG:O	2.17	0.45
1:G:65:LEU:HD23	1:G:159:LEU:C	2.36	0.45
1:A:157:THR:HG23	1:A:371:VAL:HG11	1.97	0.45
1:A:60:GLN:O	1:A:63:PRO:HD2	2.16	0.45
1:A:225:GLN:O	2:B:23:TYR:HE1	2.00	0.45
1:C:148:ILE:HG13	1:C:176:TYR:CZ	2.51	0.45
1:C:162:PHE:HB3	1:C:175:ASP:O	2.15	0.45
1:E:95:GLY:CA	1:E:135:LEU:HD11	2.44	0.45
1:A:355:TYR:CD1	1:A:355:TYR:N	2.83	0.45
1:C:154:VAL:HG11	1:C:355:TYR:CB	2.46	0.45
1:C:226:LEU:HB3	2:D:23:TYR:OH	2.17	0.45
1:C:78:GLY:O	1:C:91:CYS:HB2	2.16	0.45
1:E:162:PHE:HB3	1:E:175:ASP:O	2.15	0.45
1:E:60:GLN:OE1	1:E:390:THR:HG23	2.16	0.45
1:G:153:LEU:N	1:G:153:LEU:HD12	2.31	0.45
1:A:21:ASN:OD1	2:B:36:GLN:HB2	2.16	0.45
1:C:395:PHE:CD1	1:C:395:PHE:N	2.83	0.45
2:D:72:HIS:CD2	2:D:72:HIS:O	2.70	0.45
1:G:290:VAL:CG2	1:G:291:PRO:CD	2.94	0.45
2:H:26:LEU:HD22	2:H:41:LEU:HD21	1.98	0.45
1:A:86:GLN:HA	1:A:86:GLN:NE2	2.29	0.45
2:B:112:GLY:O	2:B:113:PRO:C	2.55	0.45
1:G:436:THR:HA	1:G:450:ILE:O	2.17	0.45
2:H:59:VAL:HG12	2:H:60:THR:N	2.31	0.45
1:A:304:TYR:CD1	1:C:303:ASN:HB3	2.52	0.45
1:A:37:GLN:C	1:A:39:PHE:N	2.70	0.45
2:B:10:ILE:O	2:B:13:PHE:HB2	2.17	0.45
2:D:3:ASP:C	2:D:5:LEU:N	2.69	0.45
2:D:85:LEU:C	2:D:85:LEU:HD12	2.36	0.45
1:E:438:CYS:SG	1:E:439:LEU:N	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:GLU:CG	2:F:97:SER:OG	2.64	0.45
1:G:303:ASN:ND2	1:G:308:GLN:HA	2.32	0.45
1:G:351:ASP:HB2	1:G:377:THR:HG21	1.99	0.45
1:G:428:VAL:HA	1:G:429:PRO:HD2	1.77	0.45
2:H:86:GLU:OE2	2:H:86:GLU:HA	2.16	0.45
1:A:24:PHE:O	2:B:135:ILE:HA	2.16	0.45
1:A:356:SER:OG	1:A:357:SER:N	2.50	0.45
1:A:86:GLN:CA	1:A:86:GLN:HE21	2.23	0.45
1:C:99:LYS:HE2	1:C:150:VAL:CG1	2.46	0.45
1:C:65:LEU:HD23	1:C:159:LEU:C	2.37	0.45
1:C:3:SER:OG	2:D:75:HIS:ND1	2.35	0.45
1:G:355:TYR:CD1	1:G:355:TYR:N	2.84	0.45
1:G:60:GLN:OE1	1:G:390:THR:HG23	2.16	0.45
1:A:148:ILE:HA	1:A:176:TYR:CE2	2.50	0.45
1:A:65:LEU:HD22	1:A:158:VAL:HG12	1.99	0.45
1:A:60:GLN:OE1	1:A:390:THR:HG23	2.16	0.45
1:A:451:SER:HB2	2:B:76:LYS:HD3	1.99	0.45
1:E:198:LEU:O	1:E:437:ALA:HB1	2.16	0.45
2:F:23:TYR:CG	2:F:24:LYS:N	2.84	0.45
1:G:212:LEU:O	1:G:213:LEU:C	2.53	0.45
1:G:37:GLN:C	1:G:39:PHE:N	2.69	0.45
1:A:360:ASP:O	1:A:363:GLU:HB3	2.16	0.45
1:C:221:VAL:HG21	1:C:452:PHE:HE2	1.81	0.45
2:H:59:VAL:O	2:H:82:GLU:HB2	2.17	0.45
1:A:277:LYS:HE2	1:A:281:GLU:CD	2.37	0.45
1:A:319:ALA:CB	1:A:325:LEU:HD22	2.46	0.45
2:B:23:TYR:CE1	2:B:38:LYS:HE2	2.52	0.45
1:C:316:PHE:O	1:C:320:THR:HG23	2.16	0.45
2:D:32:VAL:HG11	2:D:40:MET:HE1	1.98	0.45
1:C:13:LEU:HD13	2:D:38:LYS:CD	2.46	0.45
1:E:451:SER:HB2	2:F:76:LYS:HD3	1.99	0.45
1:G:280:ASP:OD1	1:G:317:PRO:HD2	2.17	0.45
1:A:136:GLU:HG2	1:A:141:ARG:HB3	1.98	0.44
1:A:218:LEU:HD22	1:A:431:PHE:CE2	2.52	0.44
1:G:373:HIS:O	1:G:376:PRO:HD3	2.17	0.44
1:A:419:GLU:O	1:A:420:ASP:C	2.55	0.44
2:B:18:ASN:OD1	2:B:105:LYS:HE2	2.17	0.44
1:C:244:ALA:HA	1:C:295:MET:HB2	1.98	0.44
1:C:303:ASN:HD21	1:C:308:GLN:HA	1.82	0.44
1:C:280:ASP:OD1	1:C:317:PRO:HD2	2.16	0.44
1:C:351:ASP:HB2	1:C:377:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLN:NE2	1:C:86:GLN:HA	2.31	0.44
1:G:360:ASP:O	1:G:363:GLU:HB3	2.17	0.44
1:A:95:GLY:CA	1:A:135:LEU:HD11	2.43	0.44
1:A:440:VAL:HG22	1:A:447:CYS:SG	2.57	0.44
1:C:198:LEU:HB3	1:C:428:VAL:HG21	1.99	0.44
2:D:103:ILE:N	2:D:104:GLN:HE21	2.14	0.44
1:E:24:PHE:CZ	1:E:233:CYS:HB2	2.52	0.44
2:F:59:VAL:O	2:F:82:GLU:HB2	2.17	0.44
1:G:26:ARG:HG3	1:G:27:VAL:H	1.81	0.44
1:G:26:ARG:NH1	1:G:289:SER:O	2.48	0.44
1:A:61:MET:HE3	1:A:158:VAL:HB	2.00	0.44
1:A:351:ASP:HB2	1:A:377:THR:HG21	1.99	0.44
1:C:444:SER:O	1:C:445:LEU:HB2	2.17	0.44
1:E:311:LEU:HA	1:E:311:LEU:HD23	1.75	0.44
1:E:418:PRO:CB	1:E:419:GLU:OE1	2.64	0.44
2:F:6:TYR:CD1	2:F:40:MET:HG2	2.52	0.44
1:G:83:CYS:HA	1:G:140:GLN:NE2	2.32	0.44
1:G:2:PHE:CG	1:G:439:LEU:HD12	2.52	0.44
1:A:99:LYS:HE2	1:A:150:VAL:HG12	1.98	0.44
1:C:37:GLN:N	1:C:37:GLN:NE2	2.64	0.44
1:C:345:SER:C	1:C:405:GLY:HA3	2.37	0.44
1:E:351:ASP:HB2	1:E:377:THR:HG21	1.98	0.44
1:G:97:LEU:CD2	1:G:133:LEU:HB3	2.47	0.44
1:G:398:CYS:SG	1:G:423:VAL:HG21	2.57	0.44
1:G:78:GLY:O	1:G:91:CYS:HB2	2.17	0.44
1:A:197:LEU:HB3	1:A:241:VAL:HG22	1.99	0.44
1:A:226:LEU:HB2	2:B:62:LEU:HD13	1.99	0.44
1:C:151:SER:CB	1:C:357:SER:HB2	2.45	0.44
1:E:61:MET:CE	1:E:158:VAL:HB	2.47	0.44
1:E:211:SER:HA	1:E:435:GLN:NE2	2.32	0.44
1:G:438:CYS:SG	1:G:439:LEU:N	2.91	0.44
2:H:125:ASN:C	2:H:127:GLN:H	2.20	0.44
1:A:398:CYS:SG	1:A:423:VAL:HG21	2.58	0.44
2:B:85:LEU:HD12	2:B:85:LEU:C	2.37	0.44
1:C:128:HIS:ND1	1:C:131:ASP:OD1	2.51	0.44
1:C:194:ARG:HG3	1:C:194:ARG:NH1	2.32	0.44
1:C:354:ARG:C	1:C:355:TYR:HD1	2.21	0.44
1:E:239:SER:O	1:E:240:ARG:HG2	2.18	0.44
1:E:303:ASN:HD22	1:E:305:THR:HG22	1.79	0.44
2:F:85:LEU:C	2:F:85:LEU:HD12	2.37	0.44
1:C:2:PHE:CG	1:C:439:LEU:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:CB	1:C:443:ARG:NH1	2.68	0.44
2:D:3:ASP:CG	2:D:4:GLN:N	2.71	0.44
2:F:122:LEU:O	2:F:126:LEU:N	2.51	0.44
2:F:70:ASN:C	2:F:72:HIS:N	2.69	0.44
1:G:354:ARG:C	1:G:355:TYR:HD1	2.21	0.44
1:A:197:LEU:HD21	1:A:218:LEU:HD11	2.00	0.44
2:B:70:ASN:C	2:B:72:HIS:H	2.21	0.44
1:E:151:SER:CB	1:E:357:SER:HB2	2.42	0.44
1:E:65:LEU:HD22	1:E:158:VAL:HG12	2.00	0.44
1:G:26:ARG:CG	1:G:27:VAL:N	2.81	0.44
1:A:148:ILE:HG13	1:A:176:TYR:CZ	2.51	0.43
1:A:185:LYS:HA	1:A:186:PRO:HD3	1.79	0.43
1:A:452:PHE:CD1	1:A:452:PHE:N	2.85	0.43
1:C:24:PHE:O	2:D:135:ILE:HA	2.18	0.43
1:C:26:ARG:HD3	1:C:290:VAL:HG23	1.98	0.43
1:E:26:ARG:CD	1:E:290:VAL:HG23	2.48	0.43
1:E:348:ASN:HB3	1:E:375:SER:HB2	1.99	0.43
1:E:440:VAL:HG22	1:E:447:CYS:SG	2.58	0.43
1:G:244:ALA:HA	1:G:295:MET:HB2	1.99	0.43
1:E:269:GLN:HE22	1:G:320:THR:HB	1.83	0.43
2:H:81:ARG:NH1	2:H:108:LEU:O	2.51	0.43
1:A:145:LYS:NZ	1:A:168:ASP:HB2	2.33	0.43
1:A:-1:HIS:ND1	1:A:-1:HIS:C	2.72	0.43
1:A:330:ASN:CB	1:A:331:PRO:HD3	2.35	0.43
1:A:284:LEU:HD23	2:B:126:LEU:HD11	2.00	0.43
1:C:308:GLN:OE1	1:C:330:ASN:ND2	2.39	0.43
1:C:342:LEU:HD12	1:C:343:GLY:H	1.83	0.43
1:C:418:PRO:CB	1:C:419:GLU:OE1	2.65	0.43
1:E:372:ARG:NH1	1:E:395:PHE:O	2.51	0.43
2:F:3:ASP:C	2:F:5:LEU:N	2.70	0.43
1:E:14:LEU:HD11	2:F:98:ILE:HG22	1.99	0.43
1:G:197:LEU:HB3	1:G:241:VAL:HG22	2.00	0.43
1:G:243:LEU:CD2	1:G:243:LEU:N	2.81	0.43
1:G:-2:HIS:O	1:G:-1:HIS:CB	2.66	0.43
1:G:37:GLN:HB2	1:G:38:PRO:CD	2.48	0.43
1:G:395:PHE:CD1	1:G:395:PHE:N	2.83	0.43
2:H:103:ILE:CA	2:H:104:GLN:HE21	2.31	0.43
1:A:162:PHE:HB3	1:A:175:ASP:O	2.17	0.43
1:A:298:GLU:OE1	1:A:298:GLU:HA	2.18	0.43
2:B:32:VAL:CG1	2:B:36:GLN:OE1	2.65	0.43
2:B:59:VAL:CG1	2:B:60:THR:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:MET:CE	1:C:158:VAL:HB	2.48	0.43
1:A:315:MET:HG2	1:C:314:CYS:SG	2.58	0.43
1:G:148:ILE:HG13	1:G:176:TYR:CZ	2.52	0.43
1:G:416:ARG:HA	1:G:421:GLN:O	2.18	0.43
1:G:443:ARG:HG2	1:G:443:ARG:HH11	1.83	0.43
1:A:85:LEU:CG	1:A:165:VAL:HG21	2.48	0.43
1:C:148:ILE:HA	1:C:176:TYR:CE2	2.49	0.43
2:D:23:TYR:CD1	2:D:34:VAL:HG22	2.53	0.43
1:E:280:ASP:CG	1:E:318:LEU:HB2	2.39	0.43
1:E:82:LEU:HD21	1:E:142:ILE:HG22	2.00	0.43
2:F:3:ASP:CG	2:F:4:GLN:N	2.72	0.43
1:G:24:PHE:O	2:H:135:ILE:HA	2.18	0.43
2:H:18:ASN:OD1	2:H:105:LYS:HE2	2.18	0.43
2:H:55:ALA:O	2:H:57:LEU:N	2.52	0.43
1:A:280:ASP:CG	1:A:318:LEU:HB2	2.38	0.43
1:A:62:ARG:CB	1:A:63:PRO:HD3	2.44	0.43
1:C:185:LYS:HG2	1:C:185:LYS:H	1.69	0.43
1:C:269:GLN:O	1:C:270:ALA:C	2.57	0.43
2:D:32:VAL:CG1	2:D:36:GLN:OE1	2.65	0.43
1:E:373:HIS:O	1:E:376:PRO:HD3	2.17	0.43
2:F:24:LYS:HB3	2:F:118:ASP:OD1	2.19	0.43
2:F:26:LEU:HD22	2:F:41:LEU:HD21	2.00	0.43
1:G:346:GLY:N	1:G:405:GLY:HA3	2.34	0.43
1:G:82:LEU:HD21	1:G:142:ILE:HG22	2.01	0.43
1:G:231:GLU:CG	2:H:97:SER:OG	2.66	0.43
1:A:154:VAL:HG11	1:A:355:TYR:CB	2.46	0.43
2:B:23:TYR:CD1	2:B:34:VAL:HG22	2.53	0.43
2:D:3:ASP:O	2:D:5:LEU:N	2.52	0.43
2:H:34:VAL:O	2:H:38:LYS:HG3	2.18	0.43
2:B:59:VAL:O	2:B:82:GLU:HB2	2.18	0.43
1:C:194:ARG:HG3	1:C:194:ARG:HH11	1.84	0.43
1:G:298:GLU:OE1	1:G:298:GLU:HA	2.18	0.43
2:H:103:ILE:C	2:H:104:GLN:HE21	2.22	0.43
1:A:239:SER:O	1:A:240:ARG:HG2	2.19	0.43
2:B:103:ILE:CA	2:B:104:GLN:HE21	2.32	0.43
2:B:17:GLN:O	2:B:18:ASN:HB2	2.18	0.43
2:B:55:ALA:O	2:B:57:LEU:N	2.52	0.43
1:C:346:GLY:N	1:C:405:GLY:HA3	2.34	0.43
1:C:365:LEU:CD1	1:C:404:CYS:HB2	2.47	0.43
1:C:80:LYS:HD3	1:C:84:GLU:HB2	2.01	0.43
2:D:4:GLN:O	2:D:8:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ASP:OD1	1:E:317:PRO:HD2	2.19	0.43
1:A:399:PRO:O	1:A:423:VAL:HG22	2.19	0.43
1:C:136:GLU:HG2	1:C:141:ARG:HB3	2.01	0.43
2:F:20:ILE:HG23	2:F:104:GLN:HG3	2.01	0.43
1:G:306:LEU:HD23	1:G:393:PHE:HE1	1.82	0.43
1:A:369:LEU:HD21	1:A:423:VAL:HG11	2.01	0.43
1:C:275:ALA:O	1:C:276:VAL:C	2.55	0.43
1:E:194:ARG:HH11	1:E:194:ARG:HG3	1.83	0.43
1:E:346:GLY:CA	1:E:405:GLY:HA3	2.48	0.43
1:G:226:LEU:HB3	2:H:23:TYR:OH	2.19	0.43
1:A:-3:HIS:CD2	1:A:-3:HIS:H1	2.37	0.42
2:B:125:ASN:C	2:B:127:GLN:H	2.22	0.42
2:B:3:ASP:C	2:B:5:LEU:N	2.72	0.42
1:A:231:GLU:CG	2:B:97:SER:OG	2.66	0.42
1:C:101:MET:HB2	1:C:128:HIS:CD2	2.54	0.42
1:C:451:SER:HB2	2:D:76:LYS:HD3	2.01	0.42
2:D:10:ILE:O	2:D:13:PHE:HB2	2.19	0.42
2:D:60:THR:OG1	2:D:102:SER:OG	2.27	0.42
1:E:86:GLN:O	1:E:87:PRO:C	2.56	0.42
1:G:128:HIS:ND1	1:G:131:ASP:OD1	2.52	0.42
1:G:145:LYS:CE	1:G:168:ASP:HB3	2.49	0.42
1:G:182:ALA:HB1	1:G:183:PRO:CD	2.39	0.42
1:G:151:SER:CB	1:G:357:SER:HB2	2.45	0.42
2:H:3:ASP:CG	2:H:4:GLN:N	2.72	0.42
1:A:151:SER:CB	1:A:357:SER:HB2	2.45	0.42
1:C:355:TYR:N	1:C:355:TYR:CD1	2.86	0.42
2:D:34:VAL:O	2:D:38:LYS:HG3	2.19	0.42
1:E:336:ILE:O	1:E:337:ASP:C	2.58	0.42
1:C:188:PRO:HD2	1:C:338:GLY:O	2.19	0.42
1:C:197:LEU:HB3	1:C:241:VAL:HG22	2.01	0.42
1:E:26:ARG:NH1	1:E:289:SER:O	2.51	0.42
2:F:18:ASN:OD1	2:F:105:LYS:HE2	2.20	0.42
1:G:125:LYS:NZ	1:G:356:SER:O	2.51	0.42
2:H:32:VAL:HG11	2:H:40:MET:HE1	2.00	0.42
2:H:59:VAL:CG1	2:H:60:THR:N	2.82	0.42
1:A:37:GLN:HB2	1:A:38:PRO:CD	2.50	0.42
1:A:395:PHE:HA	1:A:396:PRO:HD3	1.87	0.42
2:B:103:ILE:C	2:B:104:GLN:HE21	2.23	0.42
2:D:42:TYR:O	2:D:45:VAL:HG22	2.20	0.42
1:E:312:HIS:ND1	1:E:313:PRO:HD2	2.33	0.42
1:E:354:ARG:C	1:E:355:TYR:HD1	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:LEU:HD11	1:E:450:ILE:HD11	2.00	0.42
1:C:14:LEU:HA	1:C:14:LEU:HD23	1.90	0.42
1:C:190:LEU:HB2	1:C:443:ARG:HB2	2.01	0.42
1:C:312:HIS:ND1	1:C:313:PRO:HD2	2.34	0.42
1:C:342:LEU:HD12	1:C:343:GLY:N	2.34	0.42
1:E:-1:HIS:ND1	1:E:0:GLY:N	2.67	0.42
1:E:182:ALA:HB1	1:E:183:PRO:CD	2.38	0.42
1:E:209:GLY:HA2	1:E:212:LEU:HD12	2.01	0.42
1:E:277:LYS:O	1:E:280:ASP:HB3	2.20	0.42
1:E:411:GLY:HA3	1:E:427:THR:OG1	2.19	0.42
1:E:443:ARG:HH11	1:E:443:ARG:HG2	1.84	0.42
2:F:59:VAL:CG1	2:F:60:THR:N	2.81	0.42
1:G:211:SER:HA	1:G:435:GLN:NE2	2.34	0.42
1:G:307:PRO:HG3	1:G:393:PHE:HZ	1.83	0.42
1:G:346:GLY:O	1:G:347:GLN:C	2.58	0.42
1:C:145:LYS:NZ	1:C:168:ASP:CB	2.82	0.42
1:C:148:ILE:O	1:C:148:ILE:HG23	2.19	0.42
1:E:65:LEU:HD12	1:E:179:ALA:HB2	2.01	0.42
1:E:284:LEU:HD22	1:E:318:LEU:HB3	2.01	0.42
1:G:145:LYS:NZ	1:G:168:ASP:CB	2.82	0.42
1:G:86:GLN:HE21	1:G:86:GLN:CA	2.24	0.42
1:A:275:ALA:O	1:A:276:VAL:C	2.57	0.42
2:B:69:GLN:HE21	2:B:69:GLN:HB2	1.60	0.42
1:E:185:LYS:HG2	1:E:185:LYS:H	1.70	0.42
1:E:314:CYS:SG	1:G:315:MET:HG2	2.59	0.42
1:G:37:GLN:NE2	1:G:37:GLN:N	2.63	0.42
1:G:369:LEU:CD2	1:G:423:VAL:HG11	2.50	0.42
2:H:6:TYR:O	2:H:10:ILE:HG13	2.20	0.42
1:A:354:ARG:C	1:A:355:TYR:HD1	2.23	0.42
1:C:180:ASP:HA	1:C:370:ARG:O	2.20	0.42
1:C:37:GLN:HB2	1:C:38:PRO:CD	2.50	0.42
1:E:-2:HIS:O	1:E:-1:HIS:HB2	2.19	0.42
1:G:365:LEU:CD1	1:G:404:CYS:HB2	2.46	0.42
1:G:225:GLN:HE21	2:H:133:SER:HB2	1.85	0.42
2:H:21:VAL:O	2:H:102:SER:HA	2.20	0.42
1:A:101:MET:HB2	1:A:128:HIS:CD2	2.54	0.42
1:A:280:ASP:OD1	1:A:317:PRO:HD2	2.19	0.42
2:B:115:PHE:O	2:B:116:ASN:C	2.58	0.42
1:C:85:LEU:CG	1:C:165:VAL:HG21	2.50	0.42
1:C:1:MET:SD	1:C:448:GLN:HB2	2.59	0.42
2:D:103:ILE:C	2:D:104:GLN:HE21	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:ASN:C	2:D:72:HIS:N	2.72	0.42
2:D:80:VAL:HG11	2:D:88:VAL:HG21	2.01	0.42
1:E:24:PHE:O	2:F:135:ILE:HA	2.19	0.42
1:G:198:LEU:O	1:G:437:ALA:HB1	2.20	0.42
2:H:99:HIS:ND1	2:H:100:VAL:O	2.45	0.42
1:A:345:SER:C	1:A:405:GLY:HA3	2.41	0.42
1:A:82:LEU:HA	1:A:82:LEU:HD12	1.87	0.42
1:C:298:GLU:HA	1:C:298:GLU:OE1	2.20	0.42
1:C:416:ARG:HA	1:C:421:GLN:O	2.19	0.42
2:D:59:VAL:HG12	2:D:60:THR:N	2.33	0.42
1:E:149:ASP:OD2	1:E:152:LYS:HB2	2.20	0.42
2:F:69:GLN:HE21	2:F:69:GLN:HB2	1.59	0.42
1:G:101:MET:HB2	1:G:128:HIS:CD2	2.55	0.42
1:G:225:GLN:OE1	2:H:24:LYS:HE3	2.20	0.42
1:A:85:LEU:HD12	1:A:165:VAL:CG2	2.50	0.41
1:A:97:LEU:HG	1:A:159:LEU:CD2	2.47	0.41
2:B:24:LYS:HB3	2:B:118:ASP:OD1	2.20	0.41
1:C:277:LYS:HE2	1:C:281:GLU:CD	2.40	0.41
1:C:340:ARG:HB2	1:C:400:HIS:ND1	2.35	0.41
1:C:424:LEU:HD12	1:C:425:LEU:N	2.35	0.41
2:F:32:VAL:CG1	2:F:36:GLN:OE1	2.68	0.41
1:G:372:ARG:NH1	1:G:395:PHE:O	2.51	0.41
1:G:85:LEU:CG	1:G:165:VAL:HG21	2.50	0.41
2:H:64:SER:HA	2:H:76:LYS:O	2.20	0.41
1:C:153:LEU:HD12	1:C:153:LEU:N	2.35	0.41
1:C:213:LEU:O	1:C:217:LEU:HG	2.20	0.41
2:D:64:SER:HA	2:D:76:LYS:O	2.20	0.41
2:F:17:GLN:O	2:F:18:ASN:HB2	2.20	0.41
2:B:122:LEU:O	2:B:123:LYS:C	2.59	0.41
2:B:122:LEU:O	2:B:126:LEU:N	2.53	0.41
1:C:212:LEU:O	1:C:213:LEU:C	2.56	0.41
2:D:59:VAL:CG1	2:D:60:THR:N	2.82	0.41
1:E:298:GLU:HA	1:E:298:GLU:OE1	2.20	0.41
1:E:410:PHE:CD2	1:E:449:PRO:HG3	2.55	0.41
1:E:369:LEU:CD2	1:E:423:VAL:HG11	2.50	0.41
1:E:197:LEU:HA	1:E:439:LEU:HD23	2.03	0.41
1:G:14:LEU:HD11	2:H:98:ILE:HG22	2.01	0.41
1:A:410:PHE:CD2	1:A:449:PRO:HG3	2.55	0.41
1:A:77:VAL:HG13	1:A:79:VAL:CB	2.50	0.41
2:B:26:LEU:HD22	2:B:41:LEU:HD21	2.01	0.41
1:E:26:ARG:CG	1:E:27:VAL:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:SD	1:E:448:GLN:HB2	2.60	0.41
2:F:45:VAL:CG2	2:F:46:GLU:N	2.82	0.41
1:G:185:LYS:H	1:G:185:LYS:HG2	1.73	0.41
2:H:3:ASP:O	2:H:5:LEU:N	2.54	0.41
2:H:38:LYS:HD3	2:H:99:HIS:CE1	2.56	0.41
1:A:290:VAL:CG2	1:A:291:PRO:CD	2.94	0.41
1:A:351:ASP:C	1:A:353:PHE:N	2.74	0.41
1:A:180:ASP:HA	1:A:370:ARG:O	2.20	0.41
1:A:-3:HIS:H3	1:A:414:ILE:HD12	1.86	0.41
1:A:405:GLY:O	1:A:428:VAL:O	2.38	0.41
2:B:62:LEU:O	2:B:98:ILE:HA	2.20	0.41
2:F:3:ASP:O	2:F:5:LEU:N	2.54	0.41
2:H:115:PHE:O	2:H:116:ASN:C	2.58	0.41
2:H:122:LEU:O	2:H:126:LEU:N	2.54	0.41
2:H:80:VAL:HG11	2:H:88:VAL:HG21	2.03	0.41
1:A:99:LYS:HE2	1:A:150:VAL:CG1	2.50	0.41
2:D:18:ASN:OD1	2:D:105:LYS:HE2	2.20	0.41
1:E:342:LEU:HD12	1:E:343:GLY:N	2.35	0.41
1:E:37:GLN:N	1:E:37:GLN:NE2	2.67	0.41
1:G:172:LEU:CD2	3:G:474:HOH:O	2.66	0.41
1:G:410:PHE:CD2	1:G:449:PRO:HG3	2.55	0.41
2:H:32:VAL:CG1	2:H:36:GLN:OE1	2.69	0.41
2:H:23:TYR:CE1	2:H:38:LYS:HE2	2.55	0.41
2:H:3:ASP:C	2:H:5:LEU:N	2.72	0.41
1:G:3:SER:OG	2:H:75:HIS:ND1	2.37	0.41
1:A:277:LYS:O	1:A:280:ASP:HB3	2.20	0.41
1:A:391:ASP:HA	1:A:392:PRO:HD3	1.80	0.41
1:C:83:CYS:HB3	1:C:140:GLN:OE1	2.20	0.41
1:C:351:ASP:C	1:C:353:PHE:N	2.73	0.41
2:D:112:GLY:O	2:D:113:PRO:C	2.56	0.41
1:E:330:ASN:ND2	1:E:345:SER:OG	2.53	0.41
1:E:364:ILE:O	1:E:368:THR:HG23	2.20	0.41
1:G:316:PHE:O	1:G:320:THR:HG23	2.21	0.41
1:C:37:GLN:C	1:C:39:PHE:N	2.73	0.41
1:E:2:PHE:CG	1:E:439:LEU:HD12	2.56	0.41
2:F:20:ILE:HG23	2:F:104:GLN:CG	2.51	0.41
1:A:342:LEU:HD12	1:A:343:GLY:N	2.36	0.41
1:A:84:GLU:H	1:A:84:GLU:HG3	1.63	0.41
2:B:3:ASP:O	2:B:5:LEU:N	2.53	0.41
1:C:135:LEU:HB2	1:C:144:LEU:HD11	2.03	0.41
1:C:24:PHE:CZ	1:C:233:CYS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASP:CG	1:C:318:LEU:HB2	2.40	0.41
1:G:225:GLN:NE2	2:H:133:SER:HB2	2.35	0.41
1:A:82:LEU:HD21	1:A:142:ILE:HG22	2.02	0.41
1:A:346:GLY:N	1:A:405:GLY:HA3	2.36	0.41
1:A:364:ILE:O	1:A:367:TRP:HB3	2.20	0.41
1:C:229:GLU:OE2	1:E:9:ARG:NH1	2.52	0.41
1:C:333:GLN:HG3	1:C:342:LEU:HD13	2.02	0.41
1:E:353:PHE:CD1	1:E:353:PHE:C	2.94	0.41
1:E:378:ALA:HA	1:E:379:PRO:HD3	1.77	0.41
1:E:226:LEU:HB3	2:F:23:TYR:OH	2.21	0.41
2:F:80:VAL:HG11	2:F:88:VAL:HG21	2.03	0.41
1:G:77:VAL:HG13	1:G:79:VAL:CB	2.51	0.41
1:A:269:GLN:O	1:A:270:ALA:C	2.60	0.41
1:C:145:LYS:CE	1:C:168:ASP:HB3	2.51	0.41
1:C:348:ASN:HB3	1:C:375:SER:HB2	2.03	0.41
1:G:14:LEU:HA	1:G:14:LEU:HD23	1.88	0.41
1:G:145:LYS:HZ1	1:G:168:ASP:CB	2.33	0.41
1:A:197:LEU:HD13	1:A:439:LEU:HD23	2.03	0.40
2:B:45:VAL:CG2	2:B:46:GLU:N	2.84	0.40
2:B:4:GLN:O	2:B:8:GLU:HG3	2.21	0.40
1:C:185:LYS:HA	1:C:186:PRO:HD3	1.80	0.40
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.73	0.40
1:C:430:ASP:OD1	1:C:432:SER:HB3	2.21	0.40
1:C:82:LEU:HD21	1:C:142:ILE:HG22	2.03	0.40
2:D:125:ASN:O	2:D:126:LEU:C	2.58	0.40
1:E:159:LEU:CD2	1:E:159:LEU:H	2.27	0.40
1:G:277:LYS:O	1:G:281:GLU:HG3	2.21	0.40
2:H:70:ASN:O	2:H:72:HIS:N	2.54	0.40
1:A:195:PHE:HB2	1:A:238:VAL:HG22	2.03	0.40
1:A:458:GLU:HG2	1:A:459:ASP:N	2.36	0.40
1:C:369:LEU:CD2	1:C:423:VAL:HG11	2.51	0.40
1:C:198:LEU:O	1:C:437:ALA:HB1	2.21	0.40
1:C:61:MET:O	1:C:62:ARG:C	2.58	0.40
1:C:80:LYS:HD2	1:C:84:GLU:O	2.21	0.40
2:D:3:ASP:C	2:D:5:LEU:H	2.25	0.40
1:E:61:MET:O	1:E:62:ARG:C	2.60	0.40
1:E:21:ASN:OD1	2:F:36:GLN:HB2	2.21	0.40
1:G:126:TYR:HD2	1:G:355:TYR:CE1	2.34	0.40
1:A:312:HIS:ND1	1:A:313:PRO:HD2	2.36	0.40
1:A:340:ARG:HB2	1:A:400:HIS:ND1	2.36	0.40
1:A:342:LEU:O	1:A:402:TYR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LEU:C	1:C:424:LEU:HD12	2.41	0.40
1:C:197:LEU:HA	1:C:439:LEU:HD23	2.03	0.40
1:E:277:LYS:HE2	1:E:281:GLU:CD	2.40	0.40
1:E:85:LEU:CG	1:E:165:VAL:HG21	2.52	0.40
1:G:148:ILE:HG23	1:G:148:ILE:O	2.20	0.40
1:G:202:LEU:HA	1:G:202:LEU:HD23	1.89	0.40
1:G:312:HIS:ND1	1:G:313:PRO:HD2	2.36	0.40
1:G:353:PHE:CD1	1:G:353:PHE:C	2.95	0.40
1:G:82:LEU:HA	1:G:82:LEU:HD12	1.83	0.40
2:H:125:ASN:O	2:H:126:LEU:C	2.59	0.40
1:A:197:LEU:HD13	1:A:439:LEU:CD2	2.51	0.40
1:A:410:PHE:CG	1:A:449:PRO:HG3	2.57	0.40
2:B:121:ILE:HD12	2:B:121:ILE:HA	1.92	0.40
2:D:125:ASN:C	2:D:127:GLN:H	2.24	0.40
1:E:274:GLU:O	1:E:275:ALA:C	2.60	0.40
1:E:37:GLN:C	1:E:39:PHE:N	2.72	0.40
2:H:112:GLY:O	2:H:113:PRO:C	2.60	0.40
2:H:70:ASN:C	2:H:72:HIS:N	2.73	0.40
2:H:4:GLN:O	2:H:8:GLU:HG3	2.21	0.40
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.95	0.40
2:B:5:LEU:O	2:B:9:ASN:ND2	2.54	0.40
1:C:11:HIS:C	1:C:12:THR:CG2	2.89	0.40
1:C:274:GLU:O	1:C:275:ALA:C	2.59	0.40
1:C:226:LEU:HB2	2:D:62:LEU:HD13	2.03	0.40
1:E:190:LEU:HB2	1:E:443:ARG:HB2	2.02	0.40
1:E:316:PHE:O	1:E:320:THR:HG23	2.22	0.40
1:E:444:SER:O	1:E:445:LEU:HB2	2.22	0.40
1:E:7:ALA:O	1:E:9:ARG:N	2.55	0.40
2:F:137:CYS:O	2:F:138:ALA:C	2.59	0.40
1:G:306:LEU:HB3	1:G:307:PRO:CD	2.47	0.40
2:H:41:LEU:HD13	2:H:103:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/476 (85%)	321 (79%)	63 (16%)	22 (5%)	2	11
1	C	399/476 (84%)	317 (79%)	60 (15%)	22 (6%)	2	10
1	E	398/476 (84%)	325 (82%)	50 (13%)	23 (6%)	1	10
1	G	398/476 (84%)	319 (80%)	56 (14%)	23 (6%)	1	10
2	B	141/144 (98%)	110 (78%)	24 (17%)	7 (5%)	2	12
2	D	141/144 (98%)	115 (82%)	19 (14%)	7 (5%)	2	12
2	F	141/144 (98%)	113 (80%)	21 (15%)	7 (5%)	2	12
2	H	141/144 (98%)	114 (81%)	19 (14%)	8 (6%)	1	10
All	All	2165/2480 (87%)	1734 (80%)	312 (14%)	119 (6%)	2	10

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ALA
1	A	76	GLY
1	A	79	VAL
1	A	330	ASN
1	A	405	GLY
2	B	140	ALA
1	C	-1	HIS
1	C	10	ALA
1	C	76	GLY
1	C	79	VAL
1	C	330	ASN
1	C	405	GLY
2	D	140	ALA
1	E	-1	HIS
1	E	76	GLY
1	E	79	VAL
1	E	330	ASN
1	E	405	GLY
2	F	140	ALA
1	G	-1	HIS
1	G	76	GLY
1	G	79	VAL
1	G	330	ASN
1	G	405	GLY

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Mol	Chain	Res	Type
2	H	126	LEU
2	H	140	ALA
1	A	-1	HIS
1	A	8	GLN
1	A	310	PRO
1	A	420	ASP
2	B	56	GLN
2	B	84	LYS
2	B	126	LEU
1	C	8	GLN
1	C	310	PRO
1	C	420	ASP
2	D	84	LYS
2	D	126	LEU
1	E	8	GLN
1	E	10	ALA
1	E	320	THR
1	E	420	ASP
2	F	84	LYS
2	F	126	LEU
1	G	8	GLN
1	G	10	ALA
1	G	310	PRO
1	G	420	ASP
2	H	56	GLN
2	H	84	LYS
1	A	38	PRO
1	A	180	ASP
1	A	265	THR
1	A	298	GLU
1	A	305	THR
1	A	320	THR
1	C	298	GLU
1	C	305	THR
1	C	320	THR
2	D	56	GLN
1	E	38	PRO
1	E	75	SER
1	E	298	GLU
1	E	305	THR
1	E	310	PRO
2	F	56	GLN

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Mol	Chain	Res	Type
1	G	38	PRO
1	G	298	GLU
1	G	305	THR
1	G	320	THR
1	A	209	GLY
1	A	347	GLN
1	C	38	PRO
1	C	265	THR
1	C	301	PRO
1	C	347	GLN
1	E	180	ASP
1	E	301	PRO
1	G	155	THR
1	G	180	ASP
1	G	265	THR
1	G	301	PRO
1	A	155	THR
1	A	301	PRO
2	B	142	PRO
1	C	180	ASP
1	C	209	GLY
1	E	155	THR
1	E	209	GLY
1	E	265	THR
1	E	418	PRO
2	F	142	PRO
1	G	347	GLN
1	A	29	VAL
1	A	418	PRO
2	B	112	GLY
1	C	75	SER
1	C	418	PRO
2	D	142	PRO
1	E	245	GLY
1	G	29	VAL
1	G	418	PRO
2	H	142	PRO
2	B	54	GLY
1	C	29	VAL
2	F	54	GLY
1	G	245	GLY
2	H	54	GLY

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Mol	Chain	Res	Type
2	D	54	GLY
2	D	112	GLY
1	E	29	VAL
1	C	245	GLY
1	E	77	VAL
2	F	112	GLY
2	H	71	GLY
1	A	317	PRO
1	G	317	PRO
1	G	429	PRO
2	H	112	GLY

5.3.2 Protein sidechains (i)

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	355/409 (87%)	320 (90%)	35 (10%)	8 30
1	C	350/409 (86%)	318 (91%)	32 (9%)	9 34
1	E	349/409 (85%)	317 (91%)	32 (9%)	9 34
1	G	349/409 (85%)	317 (91%)	32 (9%)	9 34
2	B	125/126 (99%)	114 (91%)	11 (9%)	10 36
2	D	125/126 (99%)	115 (92%)	10 (8%)	12 40
2	F	125/126 (99%)	115 (92%)	10 (8%)	12 40
2	H	125/126 (99%)	115 (92%)	10 (8%)	12 40
All	All	1903/2140 (89%)	1731 (91%)	172 (9%)	9 35

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	8	GLN
1	A	15	SER
1	A	20	ASN

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Mol	Chain	Res	Type
1	A	21	ASN
1	A	23	THR
1	A	31	THR
1	A	37	GLN
1	A	56	THR
1	A	85	LEU
1	A	86	GLN
1	A	134	VAL
1	A	136	GLU
1	A	140	GLN
1	A	151	SER
1	A	155	THR
1	A	167	ASP
1	A	200	SER
1	A	222	VAL
1	A	226	LEU
1	A	234	SER
1	A	243	LEU
1	A	306	LEU
1	A	314	CYS
1	A	372	ARG
1	A	406	ASN
1	A	419	GLU
1	A	422	THR
1	A	430	ASP
1	A	434	THR
1	A	438	CYS
1	A	447	CYS
1	A	459	ASP
1	A	460	ASP
1	A	462	LEU
2	B	3	ASP
2	B	23	TYR
2	B	34	VAL
2	B	69	GLN
2	B	72	HIS
2	B	83	ASP
2	B	85	LEU
2	B	104	GLN
2	B	116	ASN
2	B	128	ASN
2	B	129	CYS

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Mol	Chain	Res	Type
1	C	-1	HIS
1	C	8	GLN
1	C	15	SER
1	C	20	ASN
1	C	21	ASN
1	C	23	THR
1	C	31	THR
1	C	37	GLN
1	C	56	THR
1	C	85	LEU
1	C	86	GLN
1	C	134	VAL
1	C	136	GLU
1	C	140	GLN
1	C	151	SER
1	C	155	THR
1	C	166	ARG
1	C	167	ASP
1	C	200	SER
1	C	222	VAL
1	C	226	LEU
1	C	234	SER
1	C	243	LEU
1	C	306	LEU
1	C	372	ARG
1	C	406	ASN
1	C	418	PRO
1	C	422	THR
1	C	430	ASP
1	C	434	THR
1	C	438	CYS
1	C	447	CYS
2	D	3	ASP
2	D	23	TYR
2	D	34	VAL
2	D	69	GLN
2	D	83	ASP
2	D	85	LEU
2	D	104	GLN
2	D	116	ASN
2	D	128	ASN
2	D	129	CYS

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Mol	Chain	Res	Type
1	E	-1	HIS
1	E	8	GLN
1	E	15	SER
1	E	20	ASN
1	E	21	ASN
1	E	23	THR
1	E	31	THR
1	E	37	GLN
1	E	56	THR
1	E	85	LEU
1	E	86	GLN
1	E	134	VAL
1	E	136	GLU
1	E	151	SER
1	E	155	THR
1	E	166	ARG
1	E	167	ASP
1	E	200	SER
1	E	222	VAL
1	E	226	LEU
1	E	234	SER
1	E	243	LEU
1	E	306	LEU
1	E	314	CYS
1	E	372	ARG
1	E	406	ASN
1	E	419	GLU
1	E	422	THR
1	E	430	ASP
1	E	434	THR
1	E	438	CYS
1	E	447	CYS
2	F	3	ASP
2	F	23	TYR
2	F	34	VAL
2	F	69	GLN
2	F	83	ASP
2	F	85	LEU
2	F	104	GLN
2	F	116	ASN
2	F	128	ASN
2	F	129	CYS

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Mol	Chain	Res	Type
1	G	-1	HIS
1	G	8	GLN
1	G	15	SER
1	G	20	ASN
1	G	21	ASN
1	G	23	THR
1	G	31	THR
1	G	37	GLN
1	G	56	THR
1	G	85	LEU
1	G	86	GLN
1	G	134	VAL
1	G	136	GLU
1	G	140	GLN
1	G	151	SER
1	G	155	THR
1	G	167	ASP
1	G	200	SER
1	G	222	VAL
1	G	226	LEU
1	G	234	SER
1	G	243	LEU
1	G	306	LEU
1	G	372	ARG
1	G	406	ASN
1	G	418	PRO
1	G	419	GLU
1	G	422	THR
1	G	430	ASP
1	G	434	THR
1	G	438	CYS
1	G	447	CYS
2	H	3	ASP
2	H	23	TYR
2	H	34	VAL
2	H	69	GLN
2	H	83	ASP
2	H	85	LEU
2	H	104	GLN
2	H	116	ASN
2	H	128	ASN
2	H	129	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	A	20	ASN
1	A	37	GLN
1	A	70	GLN
1	A	86	GLN
1	A	216	GLN
1	A	269	GLN
1	A	333	GLN
1	A	406	ASN
1	A	435	GLN
2	B	9	ASN
2	B	69	GLN
2	B	72	HIS
2	B	104	GLN
2	B	116	ASN
2	B	127	GLN
2	B	128	ASN
1	C	-3	HIS
1	C	20	ASN
1	C	37	GLN
1	C	70	GLN
1	C	86	GLN
1	C	216	GLN
1	C	269	GLN
1	C	285	GLN
1	C	333	GLN
1	C	406	ASN
2	D	9	ASN
2	D	69	GLN
2	D	72	HIS
2	D	104	GLN
2	D	116	ASN
2	D	127	GLN
2	D	128	ASN
1	E	-3	HIS
1	E	5	GLN
1	E	11	HIS
1	E	37	GLN
1	E	70	GLN
1	E	86	GLN
1	E	216	GLN

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Mol	Chain	Res	Type
1	E	269	GLN
1	E	326	GLN
1	E	333	GLN
1	E	406	ASN
1	E	435	GLN
2	F	9	ASN
2	F	69	GLN
2	F	104	GLN
2	F	116	ASN
2	F	127	GLN
2	F	128	ASN
1	G	-3	HIS
1	G	11	HIS
1	G	37	GLN
1	G	70	GLN
1	G	86	GLN
1	G	216	GLN
1	G	333	GLN
1	G	406	ASN
1	G	435	GLN
2	H	9	ASN
2	H	69	GLN
2	H	104	GLN
2	H	116	ASN
2	H	127	GLN
2	H	128	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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	416/476 (87%)	-0.26	4 (0%)	82	59	21, 54, 104, 113	0
1	C	409/476 (85%)	-0.34	6 (1%)	73	46	20, 50, 98, 108	0
1	E	408/476 (85%)	-0.29	8 (1%)	65	36	24, 53, 94, 107	0
1	G	408/476 (85%)	-0.15	15 (3%)	41	17	27, 58, 103, 114	0
2	B	143/144 (99%)	-0.36	3 (2%)	63	34	29, 52, 90, 113	0
2	D	143/144 (99%)	-0.41	3 (2%)	63	34	32, 49, 83, 102	0
2	F	143/144 (99%)	-0.17	2 (1%)	75	49	38, 64, 88, 116	0
2	H	143/144 (99%)	-0.12	4 (2%)	53	25	34, 68, 93, 111	0
All	All	2213/2480 (89%)	-0.26	45 (2%)	65	36	20, 56, 100, 116	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	144	ALA	5.0
2	H	144	ALA	4.1
1	A	388	TYR	3.8
1	G	265	THR	3.8
2	F	144	ALA	3.6
2	D	3	ASP	3.4
1	G	91	CYS	3.3
2	H	53	SER	3.2
1	C	265	THR	3.2
1	G	-2	HIS	3.2
1	E	128	HIS	3.2
2	H	4	GLN	3.1
1	G	128	HIS	3.1
2	F	143	ARG	2.9
2	D	71	GLY	2.8
1	E	86	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	53	SER	2.8
1	A	264	LEU	2.7
1	G	88	GLU	2.6
1	C	264	LEU	2.6
1	G	268	THR	2.6
1	A	265	THR	2.5
1	G	210	GLU	2.4
1	G	163	GLY	2.4
1	E	85	LEU	2.4
1	E	264	LEU	2.4
1	G	92	CYS	2.3
1	C	101	MET	2.3
2	D	144	ALA	2.3
2	H	55	ALA	2.3
1	G	78	GLY	2.2
1	A	131	ASP	2.2
1	C	-2	HIS	2.2
1	G	164	SER	2.2
1	G	85	LEU	2.1
1	G	207	GLY	2.1
1	E	265	THR	2.1
1	C	167	ASP	2.1
1	G	133	LEU	2.1
1	E	266	LYS	2.1
1	E	267	LYS	2.1
1	C	390	THR	2.1
1	G	127	ILE	2.0
2	B	3	ASP	2.0
1	E	126	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.