Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 05:45 pm GMT

PDB ID	:	2XLC
Title	:	Acetyl xylan esterase from Bacillus pumilus CECT5072 bound to paraoxon
Authors	:	Gil-Ortiz, F.; Montoro-Garcia, S.; Polo, L.M.; Rubio, V.; Sanchez-Ferrer, A.
Deposited on	:	2010-07-20
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

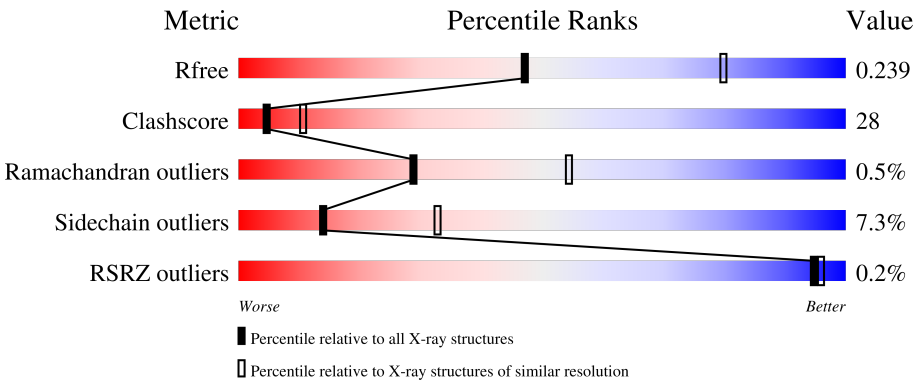
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	320	60% 33% • •
1	B	320	62% 31% 5% •
1	C	320	62% 29% 5% •
1	D	320	62% 30% 5% •
1	E	320	62% 30% 5% •

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Mol	Chain	Length	Quality of chain
1	F	320	63% 30% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DEP	A	1318	-	-	X	-
2	DEP	B	1318	-	-	X	-
2	DEP	C	1318	-	-	X	-
2	DEP	D	1318	-	-	X	-
2	DEP	E	1319	-	-	X	-
2	DEP	F	1319	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14594 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 ACETYL XYLAN ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	311	2426	1572	396	455	3	0	0	0
1	B	311	2409	1562	394	450	3	0	0	0
1	C	311	2408	1561	391	453	3	0	0	0
1	D	311	2404	1557	392	452	3	0	0	0
1	E	312	2433	1576	396	458	3	0	0	0
1	F	312	2426	1571	396	456	3	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASP	GLY	SEE REMARK 999	UNP Q9K5F2
A	236	GLU	LYS	SEE REMARK 999	UNP Q9K5F2
A	270	GLN	LYS	SEE REMARK 999	UNP Q9K5F2
A	289	GLU	ASP	SEE REMARK 999	UNP Q9K5F2
B	97	ASP	GLY	SEE REMARK 999	UNP Q9K5F2
B	236	GLU	LYS	SEE REMARK 999	UNP Q9K5F2
B	270	GLN	LYS	SEE REMARK 999	UNP Q9K5F2
B	289	GLU	ASP	SEE REMARK 999	UNP Q9K5F2
C	97	ASP	GLY	SEE REMARK 999	UNP Q9K5F2
C	236	GLU	LYS	SEE REMARK 999	UNP Q9K5F2
C	270	GLN	LYS	SEE REMARK 999	UNP Q9K5F2
C	289	GLU	ASP	SEE REMARK 999	UNP Q9K5F2
D	97	ASP	GLY	SEE REMARK 999	UNP Q9K5F2
D	236	GLU	LYS	SEE REMARK 999	UNP Q9K5F2
D	270	GLN	LYS	SEE REMARK 999	UNP Q9K5F2
D	289	GLU	ASP	SEE REMARK 999	UNP Q9K5F2
E	97	ASP	GLY	SEE REMARK 999	UNP Q9K5F2

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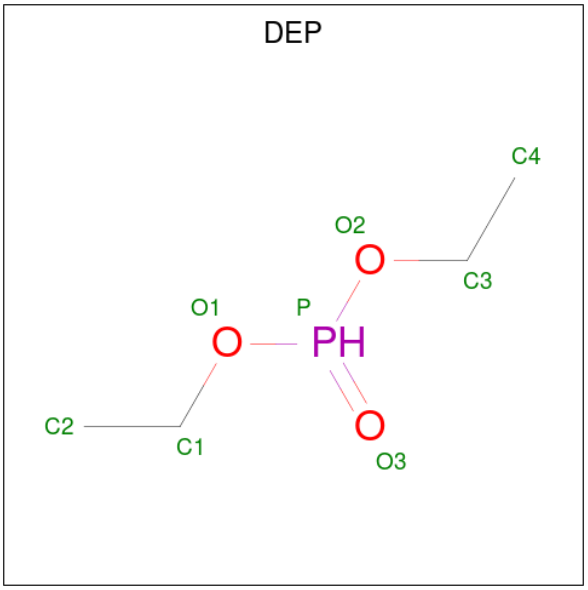
Chain	Residue	Modelled	Actual	Comment	Reference
E	236	GLU	LYS	SEE REMARK 999	UNP Q9K5F2
E	270	GLN	LYS	SEE REMARK 999	UNP Q9K5F2
E	289	GLU	ASP	SEE REMARK 999	UNP Q9K5F2
F	97	ASP	GLY	SEE REMARK 999	UNP Q9K5F2
F	236	GLU	LYS	SEE REMARK 999	UNP Q9K5F2
F	270	GLN	LYS	SEE REMARK 999	UNP Q9K5F2
F	289	GLU	ASP	SEE REMARK 999	UNP Q9K5F2

- Molecule 2 is DIETHYL PHOSPHONATE (three-letter code: DEP) (formula: $C_4H_{11}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	8	4	3	1	0	0
2	B	1	8	4	3	1	0	0
2	C	1	8	4	3	1	0	0
2	D	1	8	4	3	1	0	0
2	E	1	8	4	3	1	0	0
2	F	1	8	4	3	1	0	0

- Molecule 3 is water.

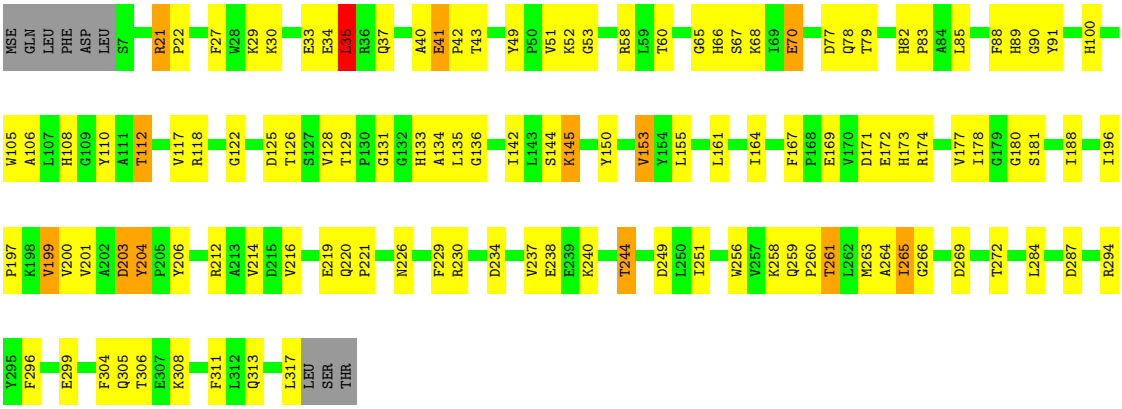
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	9	9	9	0	0
			Total	O		
3	B	11	11	11	0	0
			Total	O		
3	C	8	8	8	0	0
			Total	O		
3	D	2	2	2	0	0
			Total	O		
3	E	4	4	4	0	0
			Total	O		
3	F	6	6	6	0	0

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: ACETYL XYLAN ESTERASE

Chain A: 60% 33%

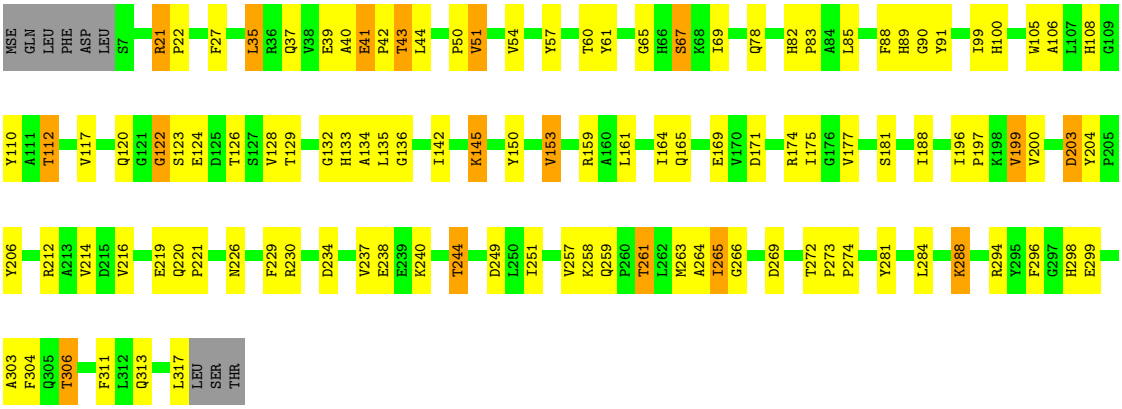


• Molecule 1: ACETYL XYLAN ESTERASE

Chain B: 62% 31% 5%

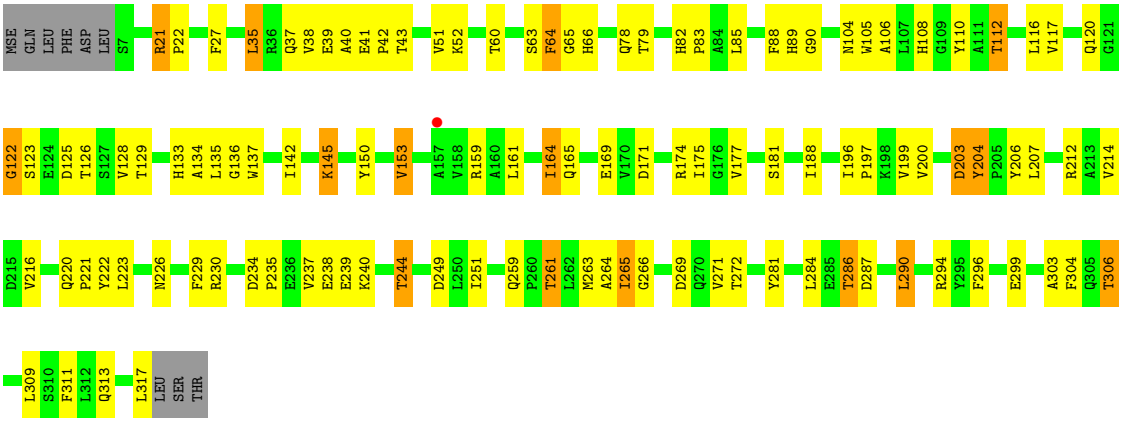
• Molecule 1: ACETYL XYLAN ESTERASE

Chain C: 62% 29% 5%



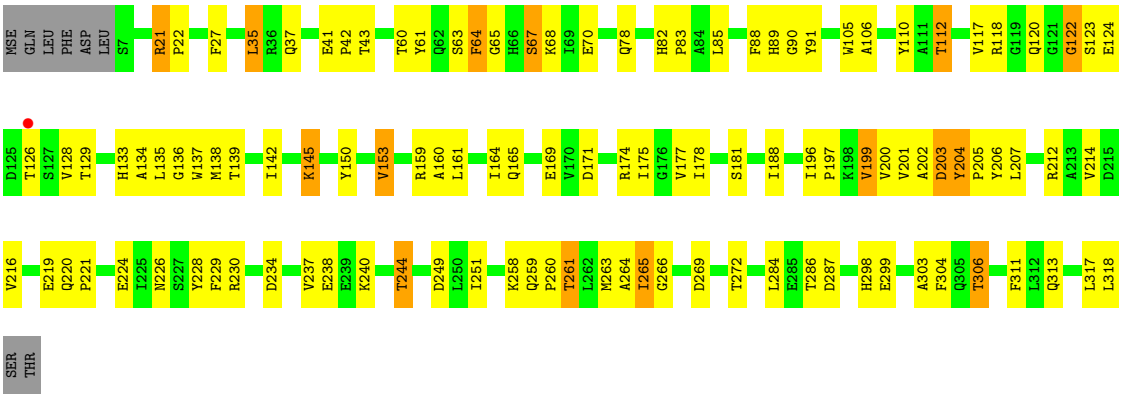
• Molecule 1: ACETYL XYLAN ESTERASE

Chain D:



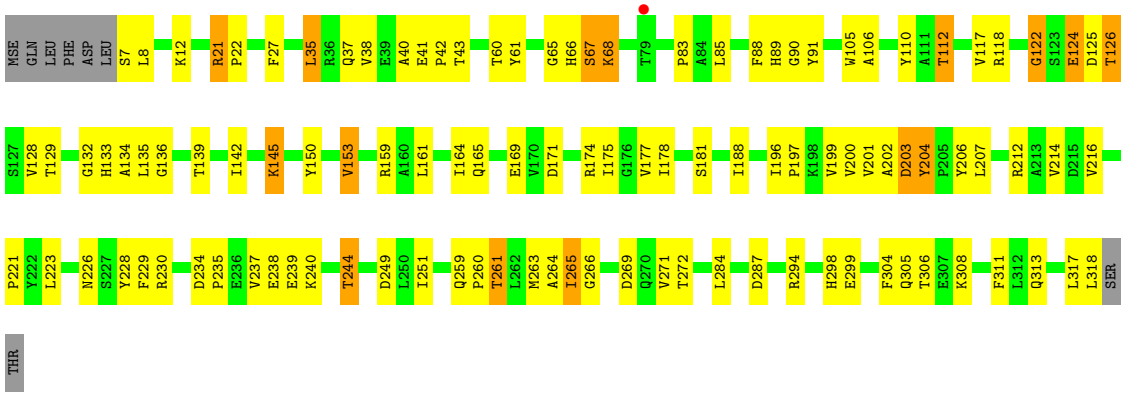
• Molecule 1: ACETYL XYLAN ESTERASE

Chain E:



• Molecule 1: ACETYL XYLAN ESTERASE

Chain F:


MSE GLN LEU PHE ASP LEU S7 L8 K12 R21 P22 F27 L35 R36 Q37 V38 E39 A40 E41 P42 T43 T60 Y61 G65 H66 S67 K68 T79 P83 A84 L85 F88 H89 G90 Y91 W105 A106 Y110 A111 T112 V117 R118 G122 S123 E124 D125 T126
S127 V128 T129 G132 H133 A134 L135 G136 T139 I142 K145 Y150 V153 R159 A160 L161 I164 Q165 E169 V170 D171 R174 I175 G176 V177 I178 S181 I188 I196 P197 K198 V199 V200 V201 A202 D203 Y204 P205 Y206 L207 R212 A213 V214 D215 V216
P221 Y222 L223 N226 S227 Y228 F229 R230 D234 P235 E236 V237 E238 E239 K240 T244 D249 L250 I251 Q259 P260 T261 L262 M263 A264 I265 G266 D269 Q270 V271 T272 L284 D287 R294 H298 E299 F304 Q305 T306 E307 K308 F311 L312 Q313 L317 L318 SER
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.05Å 116.05Å 100.25Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 74.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.70) 99.6 (74.22-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.216 , 0.236 0.215 , 0.239	Depositor DCC
R_{free} test set	2512 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14594	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 (i)

5.1 Standard geometry (i)

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

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	0.70	0/2494	0.49	1/3400 (0.0%)
1	B	0.72	0/2477	0.49	0/3380
1	C	0.65	2/2475 (0.1%)	0.50	0/3377
1	D	0.54	1/2472 (0.0%)	0.44	0/3375
1	E	0.40	0/2501	0.44	0/3411
1	F	0.42	0/2494	0.43	0/3402
All	All	0.59	3/14913 (0.0%)	0.47	1/20345 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	281	TYR	CD2-CE2	-5.34	1.31	1.39
1	D	204	TYR	CE1-CZ	-5.20	1.31	1.38
1	C	281	TYR	CE2-CZ	-5.06	1.31	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	LEU	CA-CB-CG	5.85	128.75	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2426	0	2288	152	0
1	B	2409	0	2261	128	0
1	C	2408	0	2258	145	0
1	D	2404	0	2238	147	0
1	E	2433	0	2290	143	0
1	F	2426	0	2277	142	0
2	A	8	0	10	20	0
2	B	8	0	10	17	0
2	C	8	0	10	17	0
2	D	8	0	10	10	0
2	E	8	0	10	14	0
2	F	8	0	10	17	0
3	A	9	0	0	1	0
3	B	11	0	0	1	0
3	C	8	0	0	2	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
3	F	6	0	0	0	0
All	All	14594	0	13672	797	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (797) 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:43:THR:CG2	1:F:60:THR:HB	1.67	1.23
1:F:164:ILE:HD12	1:F:165:GLN:N	1.53	1.22
1:F:221:PRO:HD2	2:F:1319:DEP:C2	1.73	1.17
1:F:181:SER:HB2	2:F:1319:DEP:H31	1.16	1.15
1:A:135:LEU:CD2	1:D:135:LEU:CD2	2.24	1.15
1:D:43:THR:CG2	1:D:60:THR:HB	1.76	1.14
1:D:43:THR:HG22	1:D:60:THR:HB	1.15	1.11
1:F:181:SER:CB	2:F:1319:DEP:C3	2.28	1.11
1:F:181:SER:HB2	2:F:1319:DEP:C3	1.80	1.10
1:C:135:LEU:CD2	1:F:135:LEU:CD2	2.30	1.09
1:B:135:LEU:CD2	1:E:135:LEU:CD2	2.30	1.09
1:A:181:SER:HB3	2:A:1318:DEP:H32	1.35	1.08
1:B:221:PRO:HD2	2:B:1318:DEP:C2	1.83	1.08
1:F:43:THR:HG22	1:F:60:THR:CB	1.84	1.08
1:C:181:SER:CB	2:C:1318:DEP:H32	1.84	1.07
1:C:181:SER:HB2	2:C:1318:DEP:H32	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:TYR:CD2	2:C:1318:DEP:H21	1.91	1.05
1:C:150:TYR:HA	1:C:153:VAL:CG1	1.87	1.04
1:E:150:TYR:HA	1:E:153:VAL:CG1	1.88	1.03
1:D:150:TYR:HA	1:D:153:VAL:CG1	1.88	1.03
1:B:150:TYR:HA	1:B:153:VAL:CG1	1.88	1.02
1:F:150:TYR:HA	1:F:153:VAL:CG1	1.89	1.01
1:B:221:PRO:HD2	2:B:1318:DEP:H23	1.07	1.01
1:E:188:ILE:HD11	1:E:263:MSE:HE2	1.40	1.01
1:A:150:TYR:HA	1:A:153:VAL:CG1	1.89	1.00
1:A:188:ILE:HD11	1:A:263:MSE:HE2	1.44	1.00
1:C:188:ILE:HD11	1:C:263:MSE:HE2	1.40	0.99
1:F:188:ILE:HD11	1:F:263:MSE:HE2	1.43	0.99
1:C:21:ARG:HG3	1:C:22:PRO:HD2	1.45	0.98
1:C:206:TYR:CE2	2:C:1318:DEP:H21	1.98	0.98
1:E:68:LYS:HD3	1:E:70:GLU:OE2	1.64	0.98
1:A:21:ARG:HG3	1:A:22:PRO:HD2	1.45	0.98
1:B:188:ILE:HD11	1:B:263:MSE:HE2	1.44	0.97
1:A:206:TYR:CE2	2:A:1318:DEP:H21	2.00	0.97
1:D:21:ARG:HG3	1:D:22:PRO:HD2	1.45	0.97
1:D:188:ILE:HD11	1:D:263:MSE:HE2	1.43	0.96
1:A:135:LEU:CD2	1:D:135:LEU:HD22	1.96	0.96
1:F:221:PRO:CD	2:F:1319:DEP:H22	1.95	0.96
1:D:43:THR:HG22	1:D:60:THR:CB	1.95	0.95
1:E:21:ARG:HG3	1:E:22:PRO:HD2	1.45	0.95
1:F:43:THR:HG22	1:F:60:THR:HB	0.97	0.95
1:F:21:ARG:HG3	1:F:22:PRO:HD2	1.46	0.94
1:D:164:ILE:HD12	1:D:164:ILE:C	1.88	0.94
1:F:221:PRO:CD	2:F:1319:DEP:C2	2.46	0.93
1:C:164:ILE:HD12	1:C:165:GLN:N	1.83	0.93
1:D:164:ILE:HD11	1:D:175:ILE:HD13	1.50	0.93
1:F:269:ASP:OD2	1:F:272:THR:HG22	1.69	0.93
1:C:269:ASP:OD2	1:C:272:THR:HG22	1.69	0.92
1:B:221:PRO:CD	2:B:1318:DEP:H23	1.97	0.92
1:A:181:SER:CB	2:A:1318:DEP:C3	2.47	0.92
1:E:204:TYR:HB2	1:E:272:THR:HG21	1.52	0.91
1:A:181:SER:HB3	2:A:1318:DEP:C3	1.99	0.91
1:D:263:MSE:HE3	1:D:284:LEU:HD11	1.49	0.91
1:F:181:SER:HB3	2:F:1319:DEP:H32	1.49	0.91
1:E:206:TYR:CG	2:E:1319:DEP:H21	2.06	0.91
1:F:313:GLN:HG3	1:F:317:LEU:HD12	1.53	0.91
1:D:269:ASP:OD2	1:D:272:THR:HG22	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASP:OD2	1:B:272:THR:HG22	1.71	0.90
1:E:164:ILE:HD12	1:E:165:GLN:N	1.85	0.90
1:A:269:ASP:OD2	1:A:272:THR:HG22	1.72	0.89
1:E:313:GLN:HG3	1:E:317:LEU:HD12	1.52	0.89
1:D:204:TYR:HB2	1:D:272:THR:HG21	1.52	0.89
1:B:313:GLN:HG3	1:B:317:LEU:HD12	1.54	0.89
1:F:181:SER:HB3	2:F:1319:DEP:C3	2.02	0.89
1:E:269:ASP:OD2	1:E:272:THR:HG22	1.72	0.89
1:A:206:TYR:CZ	2:A:1318:DEP:H21	2.07	0.88
1:C:313:GLN:HG3	1:C:317:LEU:HD12	1.54	0.88
1:F:204:TYR:HB2	1:F:272:THR:HG21	1.53	0.88
1:F:221:PRO:HD2	2:F:1319:DEP:H21	1.55	0.88
1:D:313:GLN:HG3	1:D:317:LEU:HD12	1.53	0.87
1:A:313:GLN:HG3	1:A:317:LEU:HD12	1.53	0.87
1:F:272:THR:HG23	1:F:272:THR:O	1.75	0.87
1:C:204:TYR:HB2	1:C:272:THR:HG21	1.55	0.87
1:D:272:THR:HG23	1:D:272:THR:O	1.73	0.86
1:A:272:THR:HG23	1:A:272:THR:O	1.74	0.86
1:F:181:SER:CB	2:F:1319:DEP:H31	1.97	0.86
1:D:181:SER:HB3	2:D:1318:DEP:H32	1.58	0.86
1:A:181:SER:CB	2:A:1318:DEP:H32	2.06	0.85
1:E:272:THR:HG23	1:E:272:THR:O	1.74	0.85
1:D:164:ILE:HD12	1:D:165:GLN:N	1.92	0.85
1:A:29:LYS:O	1:A:33:GLU:HG3	1.75	0.85
1:B:272:THR:O	1:B:272:THR:HG23	1.74	0.85
1:C:272:THR:HG23	1:C:272:THR:O	1.77	0.85
1:A:204:TYR:HB2	1:A:272:THR:HG21	1.59	0.85
1:E:206:TYR:CD1	2:E:1319:DEP:H21	2.12	0.84
1:A:135:LEU:HD21	1:D:135:LEU:HD22	1.60	0.83
1:A:263:MSE:HE3	1:A:284:LEU:HD11	1.57	0.83
1:B:135:LEU:CD2	1:E:135:LEU:HD22	2.07	0.83
1:C:221:PRO:HD2	2:C:1318:DEP:H11	1.61	0.83
1:A:206:TYR:CD2	2:A:1318:DEP:C2	2.62	0.82
1:C:135:LEU:CD2	1:F:135:LEU:HD22	2.09	0.82
1:A:206:TYR:CD2	2:A:1318:DEP:H21	2.15	0.81
1:A:60:THR:CG2	1:A:68:LYS:HD2	2.09	0.81
1:D:27:PHE:CE2	1:D:145:LYS:HD3	2.15	0.81
1:D:181:SER:CB	2:D:1318:DEP:H32	2.11	0.80
1:A:27:PHE:CE2	1:A:145:LYS:HD3	2.16	0.80
1:B:135:LEU:HD22	1:E:135:LEU:CD2	2.11	0.80
1:E:65:GLY:O	1:E:126:THR:HG21	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HD13	1:A:266:GLY:N	1.96	0.80
1:D:265:ILE:HD13	1:D:266:GLY:N	1.96	0.80
1:F:27:PHE:CE2	1:F:145:LYS:HD3	2.16	0.80
1:F:265:ILE:HD13	1:F:266:GLY:N	1.97	0.79
1:E:27:PHE:CE2	1:E:145:LYS:HD3	2.16	0.79
1:F:164:ILE:HD12	1:F:164:ILE:C	2.03	0.79
1:C:27:PHE:CE2	1:C:145:LYS:HD3	2.17	0.79
1:E:265:ILE:HD13	1:E:266:GLY:N	1.98	0.79
1:A:135:LEU:HD23	1:D:135:LEU:CD2	2.11	0.79
1:C:135:LEU:HD22	1:F:135:LEU:CD2	2.13	0.78
1:C:181:SER:HB3	2:C:1318:DEP:H32	1.62	0.78
1:E:21:ARG:CG	1:E:22:PRO:HD2	2.13	0.78
1:A:41:GLU:CG	1:A:41:GLU:O	2.30	0.78
1:B:164:ILE:HD13	1:B:167:PHE:CE1	2.18	0.78
1:A:181:SER:HB2	2:A:1318:DEP:C3	2.13	0.78
1:C:206:TYR:CD2	2:C:1318:DEP:C2	2.66	0.78
1:C:265:ILE:HD13	1:C:266:GLY:N	1.97	0.78
1:D:161:LEU:HD13	1:D:197:PRO:HD3	1.65	0.78
1:E:68:LYS:CD	1:E:70:GLU:OE2	2.31	0.78
1:E:181:SER:OG	2:E:1319:DEP:H22	1.84	0.77
1:A:135:LEU:CD2	1:D:135:LEU:HD21	2.12	0.77
1:A:161:LEU:HD13	1:A:197:PRO:HD3	1.66	0.77
1:E:61:TYR:CE2	1:E:159:ARG:HG2	2.19	0.77
1:A:21:ARG:CG	1:A:22:PRO:HD2	2.13	0.77
1:C:21:ARG:CG	1:C:22:PRO:HD2	2.13	0.77
1:B:265:ILE:HD13	1:B:266:GLY:N	2.00	0.77
1:F:161:LEU:HD13	1:F:197:PRO:HD3	1.66	0.77
1:B:161:LEU:HD13	1:B:197:PRO:HD3	1.67	0.77
1:C:161:LEU:HD13	1:C:197:PRO:HD3	1.66	0.77
1:A:305:GLN:NE2	1:A:308:LYS:HE3	1.98	0.77
1:B:271:VAL:HG11	2:B:1318:DEP:H12	1.67	0.77
1:A:135:LEU:HD22	1:D:135:LEU:CD2	2.12	0.76
1:B:234:ASP:HB3	1:B:237:VAL:HG23	1.67	0.76
1:C:89:HIS:CE1	1:C:117:VAL:HG23	2.19	0.76
1:E:181:SER:OG	2:E:1319:DEP:C2	2.33	0.76
1:D:120:GLN:HB3	1:D:137:TRP:CZ2	2.20	0.76
1:F:21:ARG:CG	1:F:22:PRO:HD2	2.15	0.76
1:F:181:SER:CB	2:F:1319:DEP:H32	2.07	0.75
1:E:161:LEU:HD13	1:E:197:PRO:HD3	1.66	0.75
1:D:21:ARG:CG	1:D:22:PRO:HD2	2.14	0.75
1:E:105:TRP:HB3	1:E:112:THR:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLU:O	1:A:41:GLU:HG3	1.86	0.75
1:C:181:SER:CB	2:C:1318:DEP:C3	2.62	0.75
1:D:105:TRP:HB3	1:D:112:THR:HG21	1.67	0.74
1:F:150:TYR:HA	1:F:153:VAL:HG13	1.69	0.74
1:C:150:TYR:HA	1:C:153:VAL:HG13	1.69	0.74
1:C:105:TRP:HB3	1:C:112:THR:HG21	1.68	0.74
1:F:164:ILE:HD11	1:F:175:ILE:HD13	1.70	0.74
1:E:263:MSE:HE3	1:E:284:LEU:HD11	1.68	0.74
1:F:105:TRP:HB3	1:F:112:THR:HG21	1.70	0.74
1:C:135:LEU:HD21	1:F:135:LEU:CD2	2.16	0.74
1:E:188:ILE:CD1	1:E:263:MSE:HE2	2.17	0.74
1:A:150:TYR:HA	1:A:153:VAL:HG13	1.70	0.73
1:A:110:TYR:O	1:A:112:THR:HG22	1.88	0.73
1:C:43:THR:HG22	1:C:43:THR:O	1.87	0.73
1:B:206:TYR:CE2	2:B:1318:DEP:H22	2.23	0.73
1:A:135:LEU:HD21	1:D:135:LEU:CD2	2.14	0.73
1:C:188:ILE:CD1	1:C:263:MSE:HE2	2.18	0.73
1:B:105:TRP:HB3	1:B:112:THR:HG21	1.70	0.73
1:D:206:TYR:CE2	2:D:1318:DEP:H21	2.24	0.73
1:B:271:VAL:CG1	2:B:1318:DEP:H12	2.18	0.73
1:A:41:GLU:N	1:A:42:PRO:HD3	2.04	0.72
1:A:60:THR:HG21	1:A:68:LYS:HD2	1.71	0.72
1:D:150:TYR:HA	1:D:153:VAL:HG13	1.71	0.72
1:C:284:LEU:O	1:C:288:LYS:HE2	1.88	0.72
1:E:206:TYR:CG	2:E:1319:DEP:C2	2.71	0.72
1:B:204:TYR:HB2	1:B:272:THR:HG21	1.70	0.72
1:F:235:PRO:O	1:F:239:GLU:HG3	1.89	0.72
1:E:110:TYR:O	1:E:112:THR:HG22	1.90	0.72
1:E:272:THR:O	1:E:272:THR:CG2	2.38	0.72
1:B:272:THR:O	1:B:272:THR:CG2	2.38	0.71
1:E:41:GLU:HG3	1:E:41:GLU:O	1.90	0.71
1:E:150:TYR:HA	1:E:153:VAL:HG13	1.70	0.71
1:F:68:LYS:N	1:F:124:GLU:OE1	2.18	0.71
1:D:110:TYR:O	1:D:112:THR:HG22	1.89	0.71
1:B:135:LEU:CD2	1:E:135:LEU:HD21	2.21	0.71
1:C:181:SER:HB2	2:C:1318:DEP:C3	2.16	0.71
1:A:105:TRP:HB3	1:A:112:THR:HG21	1.70	0.71
1:A:181:SER:HB2	2:A:1318:DEP:H31	1.73	0.71
1:B:150:TYR:HA	1:B:153:VAL:HG13	1.70	0.71
1:D:272:THR:O	1:D:272:THR:CG2	2.38	0.71
1:B:263:MSE:HE3	1:B:284:LEU:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:CD2	1:F:135:LEU:HD21	2.18	0.71
1:C:234:ASP:O	1:C:237:VAL:HB	1.91	0.71
1:C:135:LEU:HD21	1:F:135:LEU:HD22	1.72	0.71
1:C:164:ILE:HD11	1:C:175:ILE:HD13	1.72	0.71
1:A:272:THR:O	1:A:272:THR:CG2	2.39	0.71
1:F:110:TYR:O	1:F:112:THR:HG22	1.90	0.71
1:A:27:PHE:CD2	1:A:145:LYS:HD3	2.26	0.70
1:B:110:TYR:O	1:B:112:THR:HG22	1.90	0.70
1:B:135:LEU:HD23	1:E:135:LEU:CD2	2.21	0.70
1:A:188:ILE:CD1	1:A:263:MSE:HE2	2.21	0.70
1:B:135:LEU:HD21	1:E:135:LEU:CD2	2.20	0.70
1:C:110:TYR:O	1:C:112:THR:HG22	1.90	0.70
1:E:206:TYR:CD2	2:E:1319:DEP:H21	2.25	0.70
1:E:203:ASP:O	1:E:204:TYR:C	2.30	0.70
1:F:272:THR:O	1:F:272:THR:CG2	2.40	0.70
1:F:188:ILE:CD1	1:F:263:MSE:HE2	2.21	0.69
1:A:206:TYR:CG	2:A:1318:DEP:C2	2.76	0.69
1:F:27:PHE:CD2	1:F:145:LYS:HD3	2.28	0.69
1:E:27:PHE:CD2	1:E:145:LYS:HD3	2.26	0.69
1:A:305:GLN:NE2	1:A:308:LYS:CE	2.55	0.69
1:B:271:VAL:HG12	2:B:1318:DEP:H21	1.73	0.69
1:D:164:ILE:C	1:D:164:ILE:CD1	2.60	0.69
1:F:89:HIS:HE1	1:F:117:VAL:H	1.41	0.69
1:F:263:MSE:HE3	1:F:284:LEU:HD11	1.74	0.69
1:D:27:PHE:CD2	1:D:145:LYS:HD3	2.27	0.69
1:E:89:HIS:HE1	1:E:117:VAL:H	1.41	0.69
1:C:164:ILE:HD12	1:C:164:ILE:C	2.12	0.69
1:D:188:ILE:CD1	1:D:263:MSE:HE2	2.22	0.69
1:B:271:VAL:CG1	2:B:1318:DEP:C2	2.70	0.69
1:C:27:PHE:CD2	1:C:145:LYS:HD3	2.28	0.69
1:D:105:TRP:CB	1:D:112:THR:HG21	2.23	0.69
1:C:272:THR:O	1:C:272:THR:CG2	2.41	0.68
1:B:188:ILE:CD1	1:B:263:MSE:HE2	2.22	0.68
1:B:89:HIS:HE1	1:B:117:VAL:H	1.42	0.68
1:E:200:VAL:HB	1:E:261:THR:HB	1.76	0.68
1:A:200:VAL:HB	1:A:261:THR:HB	1.77	0.67
1:D:181:SER:CB	2:D:1318:DEP:C3	2.73	0.67
1:E:105:TRP:CB	1:E:112:THR:HG21	2.24	0.67
1:A:105:TRP:CB	1:A:112:THR:HG21	2.24	0.67
1:A:206:TYR:CE1	2:A:1318:DEP:H21	2.29	0.67
1:D:65:GLY:O	1:D:66:HIS:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:GLU:O	1:E:41:GLU:CG	2.41	0.67
1:E:240:LYS:O	1:E:244:THR:HG23	1.94	0.67
1:B:181:SER:CB	2:B:1318:DEP:H42	2.25	0.67
1:C:135:LEU:HD23	1:F:135:LEU:CD2	2.25	0.67
1:E:41:GLU:N	1:E:42:PRO:HD3	2.09	0.67
1:F:199:VAL:HG13	1:F:311:PHE:HE2	1.59	0.67
1:A:89:HIS:HE1	1:A:117:VAL:H	1.40	0.67
1:C:43:THR:HG22	1:C:60:THR:HB	1.77	0.67
1:C:199:VAL:HG13	1:C:311:PHE:HE2	1.59	0.67
1:C:263:MSE:HE3	1:C:284:LEU:HD11	1.76	0.67
1:E:199:VAL:HG13	1:E:311:PHE:HE2	1.59	0.67
1:F:200:VAL:HB	1:F:261:THR:HB	1.77	0.67
1:F:271:VAL:CG1	2:F:1319:DEP:H23	2.25	0.67
1:A:60:THR:HG23	1:A:68:LYS:HD2	1.77	0.66
1:D:264:ALA:HB2	1:D:304:PHE:CE1	2.30	0.66
1:C:200:VAL:HB	1:C:261:THR:HB	1.77	0.66
1:B:135:LEU:HD21	1:E:135:LEU:HD22	1.75	0.66
1:F:105:TRP:CB	1:F:112:THR:HG21	2.24	0.66
1:B:65:GLY:O	1:B:126:THR:HG21	1.95	0.66
1:B:105:TRP:CB	1:B:112:THR:HG21	2.25	0.66
1:B:150:TYR:HA	1:B:153:VAL:HG12	1.77	0.66
1:F:65:GLY:O	1:F:126:THR:HG21	1.95	0.66
1:A:172:GLU:HG2	1:A:173:HIS:CD2	2.30	0.66
1:B:200:VAL:HB	1:B:261:THR:HB	1.77	0.66
1:D:199:VAL:HG13	1:D:311:PHE:HE2	1.60	0.66
1:C:65:GLY:O	1:C:126:THR:HG21	1.96	0.66
1:F:221:PRO:HD3	2:F:1319:DEP:H22	1.77	0.65
1:B:199:VAL:HG13	1:B:311:PHE:HE2	1.61	0.65
1:B:240:LYS:O	1:B:244:THR:HG23	1.96	0.65
1:A:206:TYR:CE2	2:A:1318:DEP:C2	2.78	0.65
1:D:264:ALA:HB2	1:D:304:PHE:CD1	2.32	0.65
1:D:206:TYR:CD2	2:D:1318:DEP:H21	2.32	0.64
1:D:286:THR:OG1	1:D:287:ASP:N	2.30	0.64
1:A:135:LEU:HD22	1:D:135:LEU:HD21	1.78	0.64
1:A:199:VAL:HG13	1:A:311:PHE:HE2	1.62	0.64
1:D:200:VAL:HB	1:D:261:THR:HB	1.78	0.64
1:A:43:THR:HB	1:A:60:THR:HB	1.79	0.64
1:C:240:LYS:O	1:C:244:THR:HG23	1.97	0.64
1:D:203:ASP:OD2	1:D:203:ASP:N	2.30	0.64
1:C:89:HIS:HE1	1:C:117:VAL:H	1.45	0.64
1:A:230:ARG:NH2	1:C:299:GLU:OE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:HIS:HE1	1:D:117:VAL:H	1.43	0.63
1:E:206:TYR:CD1	2:E:1319:DEP:C2	2.81	0.63
1:A:144:SER:HB3	3:A:2005:HOH:O	1.98	0.63
1:F:240:LYS:O	1:F:244:THR:HG23	1.98	0.63
1:E:68:LYS:CE	1:E:70:GLU:OE2	2.46	0.63
1:A:79:THR:HG23	1:A:79:THR:O	1.96	0.63
1:A:88:PHE:HE1	1:A:177:VAL:CG2	2.12	0.63
1:F:150:TYR:HA	1:F:153:VAL:HG12	1.79	0.63
1:C:43:THR:O	1:C:43:THR:CG2	2.47	0.63
1:A:240:LYS:O	1:A:244:THR:HG23	1.98	0.63
1:B:135:LEU:CD2	1:E:135:LEU:HD23	2.25	0.62
1:C:150:TYR:HA	1:C:153:VAL:HG12	1.77	0.62
1:D:240:LYS:O	1:D:244:THR:HG23	1.99	0.62
1:A:150:TYR:HA	1:A:153:VAL:HG12	1.78	0.62
1:B:27:PHE:CD2	1:B:145:LYS:HD3	2.34	0.62
1:D:203:ASP:O	1:D:204:TYR:C	2.36	0.62
1:E:150:TYR:HA	1:E:153:VAL:HG12	1.77	0.62
1:E:181:SER:HB3	2:E:1319:DEP:H32	1.80	0.62
1:F:206:TYR:CE2	2:F:1319:DEP:H21	2.34	0.62
1:D:88:PHE:HE1	1:D:177:VAL:CG2	2.12	0.62
1:F:203:ASP:OD2	1:F:203:ASP:N	2.31	0.62
1:B:271:VAL:CG1	2:B:1318:DEP:H21	2.30	0.62
1:B:271:VAL:HG12	2:B:1318:DEP:C2	2.30	0.62
1:E:61:TYR:CD2	1:E:159:ARG:HG2	2.35	0.62
1:C:43:THR:CG2	1:C:60:THR:HB	2.30	0.61
1:D:150:TYR:HA	1:D:153:VAL:HG12	1.75	0.61
1:C:88:PHE:HE1	1:C:177:VAL:CG2	2.12	0.61
1:A:135:LEU:HD22	1:D:135:LEU:HD22	1.80	0.61
1:C:181:SER:OG	2:C:1318:DEP:H23	2.00	0.61
1:E:88:PHE:HE1	1:E:177:VAL:CG2	2.14	0.61
1:B:135:LEU:HD22	1:E:135:LEU:HD21	1.80	0.61
1:F:89:HIS:CE1	1:F:117:VAL:H	2.18	0.61
1:D:164:ILE:CD1	1:D:175:ILE:HD13	2.27	0.61
1:E:89:HIS:CE1	1:E:117:VAL:H	2.18	0.61
1:D:206:TYR:OH	1:D:221:PRO:HG2	2.01	0.61
1:C:89:HIS:HD2	1:C:90:GLY:O	1.84	0.61
1:C:135:LEU:CD2	1:F:135:LEU:HD23	2.28	0.61
1:E:89:HIS:HD2	1:E:90:GLY:O	1.84	0.61
1:A:42:PRO:HA	1:A:60:THR:O	2.01	0.61
1:B:89:HIS:CE1	1:B:117:VAL:H	2.19	0.61
1:F:61:TYR:CE2	1:F:159:ARG:HG2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:SER:HB3	2:D:1318:DEP:C3	2.29	0.61
1:E:317:LEU:O	1:E:318:LEU:C	2.39	0.60
1:D:181:SER:HB2	2:D:1318:DEP:C3	2.32	0.60
1:B:88:PHE:HE1	1:B:177:VAL:CG2	2.14	0.60
1:B:264:ALA:HB2	1:B:304:PHE:CE1	2.37	0.60
1:C:135:LEU:HD22	1:F:135:LEU:HD21	1.78	0.60
1:F:88:PHE:HE1	1:F:177:VAL:CG2	2.14	0.60
1:C:264:ALA:HB2	1:C:304:PHE:CE1	2.37	0.60
1:F:164:ILE:HD12	1:F:165:GLN:CA	2.30	0.60
1:A:206:TYR:CG	2:A:1318:DEP:H23	2.36	0.60
1:A:89:HIS:HD2	1:A:90:GLY:O	1.85	0.60
1:F:89:HIS:HD2	1:F:90:GLY:O	1.84	0.60
1:F:164:ILE:C	1:F:164:ILE:CD1	2.70	0.59
1:A:89:HIS:CE1	1:A:117:VAL:H	2.19	0.59
1:E:164:ILE:HD12	1:E:164:ILE:C	2.22	0.59
1:B:181:SER:HB2	2:B:1318:DEP:H42	1.85	0.59
1:D:89:HIS:HD2	1:D:90:GLY:O	1.85	0.59
1:E:219:GLU:HG3	1:E:220:GLN:N	2.18	0.59
1:C:298:HIS:NE2	2:C:1318:DEP:H31	2.17	0.59
1:D:271:VAL:CG1	2:D:1318:DEP:H22	2.33	0.59
1:C:91:TYR:CD2	1:C:221:PRO:HG3	2.37	0.58
1:B:271:VAL:CG1	2:B:1318:DEP:C1	2.81	0.58
1:C:89:HIS:CE1	1:C:117:VAL:H	2.21	0.58
1:E:264:ALA:HB2	1:E:304:PHE:CD1	2.37	0.58
1:A:206:TYR:CG	2:A:1318:DEP:H21	2.39	0.58
1:C:264:ALA:HB2	1:C:304:PHE:CD1	2.38	0.58
1:F:164:ILE:CD1	1:F:175:ILE:HD13	2.32	0.58
1:B:89:HIS:HD2	1:B:90:GLY:O	1.85	0.58
1:F:41:GLU:N	1:F:42:PRO:CD	2.67	0.58
1:F:42:PRO:HA	1:F:60:THR:O	2.04	0.58
1:C:78:GLN:O	1:C:82:HIS:CE1	2.55	0.58
1:C:105:TRP:CB	1:C:112:THR:HG21	2.34	0.58
1:F:305:GLN:OE1	1:F:308:LYS:HE3	2.04	0.58
1:E:220:GLN:NE2	1:E:221:PRO:HA	2.19	0.58
1:D:89:HIS:CE1	1:D:117:VAL:H	2.20	0.58
1:D:63:SER:O	1:D:64:PHE:O	2.21	0.58
1:D:303:ALA:O	1:D:306:THR:HG23	2.04	0.57
1:A:41:GLU:N	1:A:42:PRO:CD	2.67	0.57
1:B:181:SER:HB3	2:B:1318:DEP:H42	1.85	0.57
1:D:63:SER:O	1:D:64:PHE:C	2.42	0.57
1:A:256:TRP:O	1:A:258:LYS:CD	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:O	1:A:244:THR:HG21	2.04	0.57
1:C:164:ILE:CD1	1:C:175:ILE:HD13	2.35	0.57
1:A:180:GLY:HA2	1:A:203:ASP:HB2	1.86	0.57
1:A:264:ALA:HB2	1:A:304:PHE:CE1	2.39	0.57
1:B:264:ALA:HB2	1:B:304:PHE:CD1	2.40	0.56
1:D:181:SER:HB2	2:D:1318:DEP:H32	1.87	0.56
1:A:91:TYR:CD2	1:A:221:PRO:HG3	2.40	0.56
1:D:299:GLU:OE1	1:F:230:ARG:NH2	2.38	0.56
1:A:234:ASP:HB3	1:A:237:VAL:HG23	1.88	0.56
1:D:150:TYR:CD2	1:D:153:VAL:HG11	2.41	0.56
1:D:78:GLN:O	1:D:82:HIS:CE1	2.58	0.56
1:E:206:TYR:CE1	2:E:1319:DEP:H21	2.40	0.56
1:B:78:GLN:O	1:B:82:HIS:CE1	2.58	0.56
1:D:271:VAL:HG12	2:D:1318:DEP:H22	1.87	0.56
1:E:106:ALA:HA	1:E:110:TYR:O	2.06	0.56
1:E:181:SER:CB	2:E:1319:DEP:H32	2.35	0.56
1:A:106:ALA:HA	1:A:110:TYR:O	2.06	0.56
1:C:41:GLU:N	1:C:42:PRO:CD	2.69	0.55
1:E:63:SER:OG	1:E:64:PHE:N	2.39	0.55
1:F:65:GLY:O	1:F:66:HIS:HB2	2.05	0.55
1:C:142:ILE:O	1:C:244:THR:HG21	2.07	0.55
1:E:234:ASP:HB3	1:E:237:VAL:HG23	1.89	0.55
1:A:79:THR:O	1:A:79:THR:CG2	2.55	0.55
1:B:8:LEU:HG	1:B:8:LEU:O	2.07	0.55
1:D:106:ALA:HA	1:D:110:TYR:O	2.06	0.55
1:A:203:ASP:O	1:A:204:TYR:C	2.43	0.55
1:F:305:GLN:OE1	1:F:308:LYS:CE	2.54	0.55
1:A:131:GLY:HA2	1:D:123:SER:O	2.06	0.55
1:B:150:TYR:CD2	1:B:153:VAL:HG11	2.42	0.55
1:D:220:GLN:HE21	1:D:221:PRO:HA	1.70	0.55
1:B:202:ALA:HB1	1:B:205:PRO:HG3	1.88	0.55
1:A:196:ILE:N	1:A:197:PRO:HD2	2.23	0.55
1:B:27:PHE:CE2	1:B:145:LYS:HD3	2.43	0.54
1:D:142:ILE:O	1:D:244:THR:HG21	2.07	0.54
1:E:68:LYS:HE2	1:E:70:GLU:OE2	2.08	0.54
1:F:106:ALA:HA	1:F:110:TYR:O	2.05	0.54
1:B:142:ILE:O	1:B:244:THR:HG21	2.07	0.54
1:B:164:ILE:CD1	1:B:167:PHE:CE1	2.91	0.54
1:E:150:TYR:CD2	1:E:153:VAL:HG11	2.42	0.54
1:A:299:GLU:CD	1:E:230:ARG:NH2	2.61	0.54
1:C:181:SER:HB3	2:C:1318:DEP:C3	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TYR:CE2	1:B:159:ARG:HG2	2.42	0.54
1:B:106:ALA:HA	1:B:110:TYR:O	2.07	0.54
1:D:196:ILE:N	1:D:197:PRO:HD2	2.23	0.54
1:F:203:ASP:O	1:F:204:TYR:C	2.46	0.54
1:A:125:ASP:HB3	1:D:129:THR:HB	1.90	0.54
1:B:234:ASP:HB3	1:B:237:VAL:CG2	2.36	0.54
1:C:226:ASN:O	1:C:230:ARG:HG3	2.08	0.54
1:D:65:GLY:O	1:D:126:THR:HG21	2.07	0.54
1:A:206:TYR:CD1	2:A:1318:DEP:H21	2.43	0.54
1:B:135:LEU:HB3	3:B:2004:HOH:O	2.08	0.54
1:E:181:SER:CB	2:E:1319:DEP:C3	2.86	0.54
1:C:106:ALA:HA	1:C:110:TYR:O	2.07	0.54
1:C:229:PHE:CE2	1:C:238:GLU:HA	2.42	0.54
1:F:142:ILE:O	1:F:244:THR:HG21	2.07	0.54
1:C:219:GLU:HG3	1:C:220:GLN:N	2.22	0.54
1:E:78:GLN:O	1:E:82:HIS:CE1	2.60	0.54
1:F:61:TYR:CD2	1:F:159:ARG:HG2	2.43	0.54
1:D:226:ASN:O	1:D:230:ARG:HG3	2.08	0.53
1:C:220:GLN:HB3	1:C:221:PRO:HA	1.91	0.53
1:D:234:ASP:HB3	1:D:237:VAL:HG23	1.89	0.53
1:E:142:ILE:O	1:E:244:THR:HG21	2.09	0.53
1:E:264:ALA:HB2	1:E:304:PHE:CE1	2.43	0.53
1:A:91:TYR:HB3	2:A:1318:DEP:H12	1.90	0.53
1:E:65:GLY:C	1:E:126:THR:HG21	2.29	0.53
1:F:196:ILE:N	1:F:197:PRO:HD2	2.22	0.53
1:A:135:LEU:CD2	1:D:135:LEU:HD23	2.30	0.53
1:C:203:ASP:O	1:C:204:TYR:C	2.46	0.53
1:D:42:PRO:HA	1:D:60:THR:O	2.08	0.53
1:D:181:SER:HA	1:D:204:TYR:O	2.09	0.53
1:A:65:GLY:O	1:A:126:THR:HG21	2.09	0.53
1:B:196:ILE:N	1:B:197:PRO:HD2	2.23	0.53
1:A:299:GLU:OE1	1:E:230:ARG:NH2	2.41	0.53
1:C:39:GLU:O	1:C:41:GLU:HG3	2.08	0.53
1:F:298:HIS:NE2	2:F:1319:DEP:H31	2.24	0.53
1:C:196:ILE:N	1:C:197:PRO:HD2	2.24	0.53
1:F:234:ASP:HB3	1:F:237:VAL:HG23	1.89	0.53
1:A:226:ASN:O	1:A:230:ARG:HG3	2.09	0.53
1:C:61:TYR:CE2	1:C:159:ARG:HG2	2.43	0.53
1:E:226:ASN:O	1:E:230:ARG:HG3	2.09	0.53
1:B:91:TYR:CD2	1:B:221:PRO:HG3	2.44	0.52
1:C:132:GLY:H	1:F:122:GLY:HA2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:TYR:CD2	1:C:153:VAL:HG11	2.44	0.52
1:D:43:THR:HG22	1:D:60:THR:CG2	2.40	0.52
1:E:178:ILE:HG22	1:E:201:VAL:HB	1.90	0.52
1:F:226:ASN:O	1:F:230:ARG:HG3	2.09	0.52
1:E:196:ILE:N	1:E:197:PRO:HD2	2.24	0.52
1:A:53:GLY:C	1:A:77:ASP:HB3	2.29	0.52
1:A:100:HIS:CE1	1:B:305:GLN:HB3	2.45	0.52
1:A:128:VAL:HG22	1:D:126:THR:HA	1.92	0.52
1:E:181:SER:HA	1:E:204:TYR:O	2.10	0.52
1:F:150:TYR:CD2	1:F:153:VAL:HG11	2.44	0.52
1:A:150:TYR:CD2	1:A:153:VAL:HG11	2.44	0.52
1:B:203:ASP:N	1:B:203:ASP:OD2	2.42	0.52
1:C:230:ARG:NH2	1:E:299:GLU:OE2	2.43	0.52
1:B:299:GLU:OE1	1:D:230:ARG:NH2	2.43	0.52
1:F:164:ILE:HD12	1:F:165:GLN:H	1.62	0.52
1:C:288:LYS:NZ	3:C:2007:HOH:O	2.42	0.51
1:A:65:GLY:O	1:A:66:HIS:HB2	2.10	0.51
1:D:221:PRO:C	1:D:223:LEU:N	2.64	0.51
1:A:108:HIS:HE1	1:B:104:ASN:OD1	1.92	0.51
1:F:171:ASP:OD2	1:F:174:ARG:HD3	2.10	0.51
1:F:305:GLN:OE1	1:F:305:GLN:HA	2.10	0.51
1:B:171:ASP:OD2	1:B:174:ARG:HD3	2.11	0.51
1:A:263:MSE:CE	1:A:284:LEU:HD11	2.36	0.51
1:A:299:GLU:OE2	1:E:230:ARG:NH2	2.40	0.51
1:D:39:GLU:O	1:D:41:GLU:HG2	2.11	0.51
1:C:133:HIS:HD2	1:C:134:ALA:O	1.94	0.51
1:D:133:HIS:HD2	1:D:134:ALA:O	1.93	0.51
1:E:118:ARG:HA	1:E:123:SER:HB2	1.93	0.51
1:C:257:VAL:C	1:C:258:LYS:HD2	2.32	0.51
1:A:171:ASP:OD2	1:A:174:ARG:HD3	2.11	0.50
1:C:220:GLN:NE2	3:C:2003:HOH:O	2.44	0.50
1:F:142:ILE:O	1:F:142:ILE:HG13	2.11	0.50
1:A:129:THR:HB	1:D:125:ASP:HB3	1.93	0.50
1:A:133:HIS:HD2	1:A:134:ALA:O	1.94	0.50
1:B:206:TYR:CZ	2:B:1318:DEP:H22	2.46	0.50
1:D:299:GLU:CD	1:F:230:ARG:NH2	2.64	0.50
1:A:91:TYR:CB	2:A:1318:DEP:H12	2.41	0.50
1:A:135:LEU:HD23	1:D:135:LEU:HD23	1.90	0.50
1:A:142:ILE:O	1:A:142:ILE:HG13	2.11	0.50
1:C:99:ILE:HG23	1:C:100:HIS:N	2.25	0.50
1:D:63:SER:OG	1:D:64:PHE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:HIS:HD2	1:E:134:ALA:O	1.94	0.50
1:B:133:HIS:HD2	1:B:134:ALA:O	1.94	0.50
1:B:265:ILE:HD13	1:B:266:GLY:O	2.12	0.50
1:C:142:ILE:O	1:C:142:ILE:HG13	2.11	0.50
1:E:171:ASP:OD2	1:E:174:ARG:HD3	2.11	0.50
1:B:271:VAL:HG12	2:B:1318:DEP:C1	2.40	0.50
1:D:85:LEU:HB2	1:D:112:THR:HB	1.94	0.50
1:F:40:ALA:HB1	1:F:42:PRO:HD3	1.94	0.50
1:B:135:LEU:HD23	1:E:135:LEU:HD23	1.91	0.50
1:E:91:TYR:CD2	1:E:221:PRO:HG3	2.47	0.50
1:E:142:ILE:O	1:E:142:ILE:HG13	2.12	0.50
1:D:171:ASP:OD2	1:D:174:ARG:HD3	2.12	0.49
1:D:263:MSE:CE	1:D:284:LEU:HD11	2.32	0.49
1:C:42:PRO:HA	1:C:60:THR:O	2.11	0.49
1:B:85:LEU:HB2	1:B:112:THR:HB	1.94	0.49
1:B:135:LEU:HD22	1:E:135:LEU:HD22	1.81	0.49
1:C:221:PRO:CD	2:C:1318:DEP:H11	2.40	0.49
1:A:49:TYR:O	1:A:51:VAL:N	2.45	0.49
1:C:44:LEU:CD2	1:C:57:TYR:HB3	2.43	0.49
1:E:318:LEU:C	1:E:318:LEU:HD12	2.33	0.49
1:A:264:ALA:HB2	1:A:304:PHE:CD1	2.47	0.49
1:D:206:TYR:CE2	1:D:222:TYR:CE1	3.01	0.49
1:E:303:ALA:O	1:E:306:THR:HG23	2.13	0.49
1:A:269:ASP:CG	1:A:272:THR:HG22	2.34	0.49
1:C:85:LEU:HB2	1:C:112:THR:HB	1.95	0.49
1:F:133:HIS:HD2	1:F:134:ALA:O	1.94	0.49
1:A:265:ILE:HD13	1:A:266:GLY:O	2.13	0.48
1:B:132:GLY:H	1:E:122:GLY:HA2	1.78	0.48
1:E:265:ILE:HD13	1:E:266:GLY:O	2.13	0.48
1:F:85:LEU:HB2	1:F:112:THR:HB	1.94	0.48
1:A:181:SER:OG	2:A:1318:DEP:H23	2.13	0.48
1:D:188:ILE:HD11	1:D:263:MSE:CE	2.30	0.48
1:B:164:ILE:HD13	1:B:167:PHE:HE1	1.72	0.48
1:B:259:GLN:O	1:B:261:THR:HG22	2.14	0.48
1:F:40:ALA:CB	1:F:42:PRO:HD3	2.42	0.48
1:F:126:THR:HG23	1:F:126:THR:O	2.12	0.48
1:B:35:LEU:HD22	1:B:159:ARG:CZ	2.44	0.48
1:B:215:ASP:HA	1:F:294:ARG:NH2	2.29	0.48
1:C:269:ASP:CG	1:C:272:THR:HG22	2.34	0.48
1:E:135:LEU:HD23	1:E:136:GLY:N	2.28	0.48
1:B:41:GLU:N	1:B:42:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:O	1:B:142:ILE:HG13	2.12	0.48
1:B:164:ILE:CD1	1:B:167:PHE:HE1	2.26	0.48
1:A:135:LEU:HD23	1:D:135:LEU:HD21	1.88	0.48
1:C:35:LEU:HD22	1:C:159:ARG:CZ	2.44	0.48
1:A:219:GLU:HG3	1:A:220:GLN:N	2.29	0.48
1:C:171:ASP:OD2	1:C:174:ARG:HD3	2.13	0.48
1:B:249:ASP:OD2	1:B:251:ILE:HG12	2.13	0.48
1:C:40:ALA:CB	1:C:42:PRO:HD3	2.44	0.48
1:C:44:LEU:HD23	1:C:57:TYR:HB3	1.96	0.48
1:C:181:SER:HA	1:C:204:TYR:O	2.14	0.48
1:D:142:ILE:O	1:D:142:ILE:HG13	2.14	0.48
1:F:264:ALA:HB2	1:F:304:PHE:CD1	2.49	0.48
1:A:259:GLN:O	1:A:261:THR:HG22	2.13	0.47
1:C:61:TYR:CD2	1:C:159:ARG:HG2	2.49	0.47
1:D:135:LEU:HD23	1:D:136:GLY:N	2.29	0.47
1:E:85:LEU:HB2	1:E:112:THR:HB	1.96	0.47
1:C:150:TYR:CA	1:C:153:VAL:HG13	2.41	0.47
1:E:35:LEU:HD22	1:E:159:ARG:CZ	2.44	0.47
1:F:135:LEU:HD23	1:F:136:GLY:N	2.29	0.47
1:F:259:GLN:O	1:F:261:THR:HG22	2.15	0.47
1:F:269:ASP:CG	1:F:272:THR:HG22	2.32	0.47
1:D:35:LEU:HD22	1:D:159:ARG:CZ	2.44	0.47
1:E:188:ILE:HD11	1:E:263:MSE:CE	2.29	0.47
1:A:35:LEU:HG	1:A:155:LEU:HB3	1.96	0.47
1:B:35:LEU:HD22	1:B:159:ARG:NH2	2.30	0.47
1:B:61:TYR:CD2	1:B:159:ARG:HG2	2.49	0.47
1:E:164:ILE:CD1	1:E:175:ILE:HD13	2.44	0.47
1:E:269:ASP:CG	1:E:272:THR:HG22	2.35	0.47
1:A:135:LEU:HD23	1:A:136:GLY:N	2.29	0.47
1:B:305:GLN:HA	1:B:305:GLN:OE1	2.14	0.47
1:D:269:ASP:CG	1:D:272:THR:HG22	2.33	0.47
1:E:177:VAL:HG13	1:E:177:VAL:O	2.15	0.47
1:F:67:SER:HA	1:F:124:GLU:OE1	2.14	0.47
1:F:150:TYR:CA	1:F:153:VAL:HG13	2.42	0.47
1:A:41:GLU:O	1:A:41:GLU:HG2	2.13	0.47
1:A:85:LEU:HB2	1:A:112:THR:HB	1.96	0.47
1:A:214:VAL:HG13	1:A:226:ASN:ND2	2.30	0.47
1:C:35:LEU:HD22	1:C:159:ARG:NH2	2.30	0.47
1:C:259:GLN:O	1:C:261:THR:HG22	2.14	0.47
1:D:259:GLN:O	1:D:261:THR:HG22	2.15	0.47
1:E:181:SER:HB2	2:E:1319:DEP:C3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD22	1:D:159:ARG:NH2	2.30	0.47
1:D:220:GLN:NE2	1:D:221:PRO:HA	2.30	0.47
1:C:206:TYR:CG	2:C:1318:DEP:C2	2.98	0.46
1:E:128:VAL:CG1	1:E:129:THR:N	2.78	0.46
1:E:206:TYR:OH	1:E:221:PRO:HG2	2.14	0.46
1:F:214:VAL:HG13	1:F:226:ASN:ND2	2.29	0.46
1:F:265:ILE:HD13	1:F:266:GLY:O	2.15	0.46
1:B:203:ASP:O	1:B:204:TYR:C	2.51	0.46
1:D:229:PHE:CE2	1:D:238:GLU:HA	2.50	0.46
1:C:177:VAL:HG13	1:C:177:VAL:O	2.15	0.46
1:B:135:LEU:HD23	1:B:136:GLY:N	2.30	0.46
1:C:164:ILE:HD12	1:C:165:GLN:CA	2.45	0.46
1:A:256:TRP:O	1:A:258:LYS:HD2	2.16	0.46
1:C:265:ILE:HD13	1:C:266:GLY:O	2.15	0.46
1:D:265:ILE:HD13	1:D:265:ILE:C	2.36	0.46
1:C:214:VAL:HG13	1:C:226:ASN:ND2	2.31	0.46
1:C:258:LYS:HD2	1:C:258:LYS:N	2.31	0.46
1:D:265:ILE:HD13	1:D:266:GLY:O	2.16	0.46
1:E:120:GLN:HB3	1:E:137:TRP:CH2	2.51	0.46
1:E:259:GLN:O	1:E:261:THR:HG22	2.15	0.46
1:A:229:PHE:CE2	1:A:238:GLU:HA	2.51	0.46
1:A:249:ASP:OD2	1:A:251:ILE:HG12	2.15	0.46
1:F:35:LEU:HD22	1:F:159:ARG:CZ	2.46	0.46
1:F:249:ASP:OD2	1:F:251:ILE:HG12	2.16	0.46
1:C:249:ASP:OD2	1:C:251:ILE:HG12	2.16	0.46
1:E:35:LEU:HD22	1:E:159:ARG:NH2	2.31	0.46
1:E:214:VAL:HG13	1:E:226:ASN:ND2	2.30	0.46
1:E:229:PHE:CE2	1:E:238:GLU:HA	2.51	0.46
1:F:35:LEU:HD22	1:F:159:ARG:NH2	2.31	0.46
1:A:128:VAL:CG1	1:A:129:THR:N	2.79	0.46
1:D:40:ALA:O	1:D:41:GLU:HG3	2.16	0.46
1:A:78:GLN:O	1:A:82:HIS:CE1	2.69	0.45
1:A:197:PRO:O	1:A:259:GLN:HG2	2.16	0.45
1:A:240:LYS:O	1:A:244:THR:CG2	2.65	0.45
1:C:44:LEU:CD2	1:C:57:TYR:CB	2.94	0.45
1:C:128:VAL:CG1	1:C:129:THR:N	2.79	0.45
1:D:221:PRO:C	1:D:223:LEU:H	2.19	0.45
1:E:181:SER:HB3	2:E:1319:DEP:C3	2.46	0.45
1:C:181:SER:OG	2:C:1318:DEP:C2	2.63	0.45
1:A:265:ILE:HD13	1:A:265:ILE:C	2.36	0.45
1:B:128:VAL:CG1	1:B:129:THR:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD23	1:C:136:GLY:N	2.31	0.45
1:D:150:TYR:CA	1:D:153:VAL:HG13	2.43	0.45
1:C:199:VAL:CG1	1:C:311:PHE:HE2	2.28	0.45
1:D:214:VAL:HG13	1:D:226:ASN:ND2	2.31	0.45
1:C:67:SER:HB3	1:C:126:THR:HB	1.98	0.45
1:C:265:ILE:HD13	1:C:265:ILE:C	2.37	0.45
1:D:120:GLN:HB3	1:D:137:TRP:CH2	2.52	0.45
1:B:131:GLY:HA2	1:E:123:SER:O	2.16	0.45
1:E:135:LEU:HD23	1:E:135:LEU:C	2.36	0.45
1:E:197:PRO:O	1:E:259:GLN:HG2	2.17	0.45
1:F:265:ILE:HD13	1:F:265:ILE:C	2.37	0.45
1:E:240:LYS:O	1:E:244:THR:CG2	2.64	0.45
1:F:206:TYR:CZ	2:F:1319:DEP:H21	2.52	0.45
1:D:128:VAL:CG1	1:D:129:THR:N	2.79	0.45
1:D:177:VAL:HG13	1:D:177:VAL:O	2.17	0.45
1:D:220:GLN:HE21	1:D:220:GLN:HB3	1.52	0.45
1:A:206:TYR:CD1	2:A:1318:DEP:C2	2.99	0.45
1:A:220:GLN:HB3	1:A:221:PRO:HA	1.99	0.45
1:B:150:TYR:CA	1:B:153:VAL:HG13	2.43	0.45
1:C:51:VAL:HG23	1:D:108:HIS:CD2	2.52	0.45
1:E:150:TYR:CA	1:E:153:VAL:HG13	2.42	0.45
1:F:8:LEU:O	1:F:12:LYS:HG3	2.17	0.45
1:A:40:ALA:C	1:A:42:PRO:HD3	2.36	0.45
1:A:230:ARG:NH2	1:C:299:GLU:CD	2.71	0.45
1:B:269:ASP:CG	1:B:272:THR:HG22	2.36	0.45
1:C:197:PRO:O	1:C:259:GLN:HG2	2.16	0.45
1:D:281:TYR:CE1	1:D:290:LEU:HB2	2.52	0.45
1:B:197:PRO:O	1:B:259:GLN:HG2	2.16	0.44
1:F:89:HIS:CE1	1:F:117:VAL:HG23	2.52	0.44
1:F:91:TYR:CD2	1:F:221:PRO:HG3	2.52	0.44
1:B:265:ILE:CD1	1:B:266:GLY:O	2.66	0.44
1:E:265:ILE:HD13	1:E:265:ILE:C	2.37	0.44
1:F:260:PRO:HA	1:F:287:ASP:O	2.17	0.44
1:B:226:ASN:O	1:B:230:ARG:HG3	2.18	0.44
1:C:206:TYR:CG	2:C:1318:DEP:H21	2.49	0.44
1:A:30:LYS:O	1:A:34:GLU:HG3	2.18	0.44
1:C:50:PRO:HB2	1:D:309:LEU:HB3	1.98	0.44
1:C:199:VAL:CG1	1:C:200:VAL:N	2.81	0.44
1:E:160:ALA:O	1:E:164:ILE:HG13	2.17	0.44
1:F:317:LEU:O	1:F:318:LEU:C	2.56	0.44
1:A:177:VAL:O	1:A:177:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PRO:HA	1:A:287:ASP:O	2.17	0.44
1:D:249:ASP:OD2	1:D:251:ILE:HG12	2.17	0.44
1:E:63:SER:O	1:E:64:PHE:C	2.55	0.44
1:E:265:ILE:CD1	1:E:266:GLY:O	2.66	0.44
1:F:202:ALA:O	1:F:263:MSE:HA	2.18	0.44
1:E:206:TYR:CE2	2:E:1319:DEP:H21	2.52	0.44
1:E:249:ASP:OD2	1:E:251:ILE:HG12	2.17	0.44
1:F:128:VAL:CG1	1:F:129:THR:N	2.80	0.44
1:F:197:PRO:O	1:F:259:GLN:HG2	2.18	0.44
1:C:135:LEU:HD23	1:F:135:LEU:HD23	1.96	0.44
1:D:197:PRO:O	1:D:259:GLN:HG2	2.17	0.44
1:D:299:GLU:CD	1:F:230:ARG:HH22	2.21	0.44
1:F:199:VAL:CG1	1:F:311:PHE:HE2	2.29	0.44
1:F:229:PHE:CE2	1:F:238:GLU:HA	2.53	0.44
1:B:38:VAL:O	1:B:159:ARG:NH1	2.42	0.44
1:D:65:GLY:C	1:D:126:THR:HG21	2.38	0.44
1:D:135:LEU:HD23	1:D:135:LEU:C	2.39	0.44
1:F:214:VAL:O	1:F:214:VAL:CG1	2.66	0.44
1:B:240:LYS:O	1:B:244:THR:CG2	2.64	0.44
1:D:38:VAL:O	1:D:159:ARG:NH1	2.42	0.44
1:D:78:GLN:O	1:D:82:HIS:HE1	1.99	0.44
1:E:214:VAL:O	1:E:214:VAL:CG1	2.65	0.44
1:A:135:LEU:HD23	1:A:135:LEU:C	2.37	0.43
1:C:40:ALA:C	1:C:42:PRO:HD3	2.38	0.43
1:D:206:TYR:HE2	1:D:222:TYR:CE1	2.36	0.43
1:E:219:GLU:CG	1:E:220:GLN:N	2.80	0.43
1:A:265:ILE:CD1	1:A:266:GLY:O	2.66	0.43
1:B:260:PRO:HA	1:B:287:ASP:O	2.17	0.43
1:B:305:GLN:OE1	1:B:308:LYS:CE	2.66	0.43
1:D:41:GLU:N	1:D:42:PRO:CD	2.81	0.43
1:B:199:VAL:CG1	1:B:311:PHE:HE2	2.31	0.43
1:C:188:ILE:CD1	1:C:263:MSE:CE	2.93	0.43
1:C:220:GLN:CB	1:C:221:PRO:HA	2.45	0.43
1:B:177:VAL:HG13	1:B:177:VAL:O	2.19	0.43
1:B:199:VAL:CG1	1:B:200:VAL:N	2.81	0.43
1:C:273:PRO:HA	1:C:274:PRO:HD3	1.96	0.43
1:D:212:ARG:CZ	1:D:216:VAL:HG21	2.48	0.43
1:E:220:GLN:HA	1:E:221:PRO:HA	1.73	0.43
1:F:135:LEU:HD23	1:F:135:LEU:C	2.39	0.43
1:C:83:PRO:HG3	1:C:317:LEU:HD23	2.00	0.43
1:E:188:ILE:CD1	1:E:263:MSE:CE	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:GLN:HE21	1:E:221:PRO:HA	1.84	0.43
1:A:51:VAL:HG22	1:A:52:LYS:N	2.34	0.43
1:A:214:VAL:O	1:A:214:VAL:CG1	2.66	0.43
1:B:199:VAL:HG13	1:B:200:VAL:N	2.34	0.43
1:D:40:ALA:C	1:D:41:GLU:CG	2.86	0.43
1:A:29:LYS:O	1:A:33:GLU:CG	2.57	0.43
1:D:164:ILE:HD12	1:D:165:GLN:CA	2.48	0.43
1:E:43:THR:HB	1:E:60:THR:HB	2.01	0.43
1:E:260:PRO:HA	1:E:287:ASP:O	2.18	0.43
1:F:178:ILE:HG22	1:F:201:VAL:HB	2.01	0.43
1:F:199:VAL:CG1	1:F:200:VAL:N	2.82	0.43
1:A:67:SER:OG	1:A:126:THR:HG22	2.19	0.43
1:B:230:ARG:HH22	1:F:299:GLU:CD	2.21	0.43
1:C:240:LYS:O	1:C:244:THR:CG2	2.65	0.43
1:D:116:LEU:HD13	1:D:122:GLY:HA3	2.01	0.43
1:E:41:GLU:N	1:E:42:PRO:CD	2.78	0.43
1:B:305:GLN:OE1	1:B:308:LYS:HE3	2.19	0.43
1:D:214:VAL:O	1:D:214:VAL:CG1	2.66	0.43
1:F:105:TRP:HB2	1:F:112:THR:HG21	2.01	0.43
1:F:118:ARG:HB2	1:F:125:ASP:HB2	2.01	0.43
1:F:177:VAL:O	1:F:177:VAL:HG13	2.19	0.43
1:C:122:GLY:HA2	1:F:132:GLY:H	1.84	0.42
1:B:135:LEU:HD23	1:B:135:LEU:C	2.39	0.42
1:C:199:VAL:HG13	1:C:200:VAL:N	2.34	0.42
1:F:212:ARG:CZ	1:F:216:VAL:HG21	2.49	0.42
1:A:294:ARG:HD2	1:A:294:ARG:O	2.20	0.42
1:B:212:ARG:NH2	1:B:216:VAL:HG21	2.34	0.42
1:C:294:ARG:HD2	1:C:294:ARG:O	2.19	0.42
1:E:120:GLN:HB3	1:E:137:TRP:CZ2	2.55	0.42
1:F:298:HIS:NE2	2:F:1319:DEP:C3	2.83	0.42
1:C:67:SER:HB2	1:C:124:GLU:O	2.18	0.42
1:E:272:THR:HG22	1:E:298:HIS:HD1	1.84	0.42
1:A:150:TYR:CA	1:A:153:VAL:HG13	2.42	0.42
1:A:212:ARG:CZ	1:A:216:VAL:HG21	2.49	0.42
1:D:51:VAL:HG22	1:D:52:LYS:N	2.35	0.42
1:A:299:GLU:CD	1:E:230:ARG:HH22	2.21	0.42
1:C:214:VAL:O	1:C:214:VAL:CG1	2.67	0.42
1:D:199:VAL:CG1	1:D:200:VAL:N	2.82	0.42
1:D:294:ARG:HD2	1:D:294:ARG:O	2.20	0.42
1:E:67:SER:HB3	1:E:124:GLU:O	2.19	0.42
1:E:199:VAL:HG13	1:E:311:PHE:CE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:O	1:B:165:GLN:HG2	2.19	0.42
1:B:294:ARG:HD2	1:B:294:ARG:O	2.19	0.42
1:C:100:HIS:CE1	1:D:306:THR:HG22	2.55	0.42
1:C:265:ILE:CD1	1:C:266:GLY:O	2.68	0.42
1:C:135:LEU:HD23	1:C:135:LEU:C	2.39	0.42
1:A:214:VAL:O	1:A:214:VAL:HG12	2.20	0.42
1:B:18:LYS:HB3	1:B:252:ASN:OD1	2.19	0.42
1:B:178:ILE:HG22	1:B:201:VAL:HB	2.02	0.42
1:B:265:ILE:HD13	1:B:265:ILE:C	2.40	0.42
1:D:214:VAL:O	1:D:214:VAL:HG12	2.20	0.42
1:E:212:ARG:CZ	1:E:216:VAL:HG21	2.49	0.42
1:C:40:ALA:O	1:C:41:GLU:C	2.57	0.41
1:D:83:PRO:HG3	1:D:317:LEU:HD23	2.02	0.41
1:D:235:PRO:O	1:D:239:GLU:HG3	2.19	0.41
1:D:265:ILE:CD1	1:D:266:GLY:O	2.68	0.41
1:F:265:ILE:CD1	1:F:266:GLY:O	2.68	0.41
1:F:188:ILE:HD11	1:F:263:MSE:CE	2.32	0.41
1:A:77:ASP:C	1:A:77:ASP:OD1	2.57	0.41
1:A:199:VAL:CG1	1:A:200:VAL:N	2.82	0.41
1:A:220:GLN:HA	1:A:221:PRO:HA	1.85	0.41
1:B:118:ARG:HA	1:B:123:SER:HB2	2.03	0.41
1:B:139:THR:HG21	1:B:228:TYR:HB2	2.02	0.41
1:E:219:GLU:HG3	1:E:220:GLN:H	1.84	0.41
1:F:83:PRO:HG3	1:F:317:LEU:HD23	2.01	0.41
1:F:188:ILE:CD1	1:F:263:MSE:CE	2.96	0.41
1:A:178:ILE:HG22	1:A:201:VAL:HB	2.02	0.41
1:A:188:ILE:CD1	1:A:263:MSE:CE	2.95	0.41
1:B:271:VAL:HG12	2:B:1318:DEP:H12	1.97	0.41
1:C:212:ARG:CZ	1:C:216:VAL:HG21	2.50	0.41
1:D:266:GLY:HA3	1:D:296:PHE:O	2.20	0.41
1:A:83:PRO:HG3	1:A:317:LEU:HD23	2.02	0.41
1:B:206:TYR:OH	1:B:221:PRO:HG2	2.20	0.41
1:D:65:GLY:HA3	1:D:126:THR:HG21	2.02	0.41
1:F:43:THR:CG2	1:F:60:THR:CB	2.61	0.41
1:A:118:ARG:O	1:A:118:ARG:HG3	2.21	0.41
1:A:164:ILE:HA	1:A:167:PHE:CD1	2.55	0.41
1:E:202:ALA:HB1	1:E:205:PRO:HG3	2.02	0.41
1:F:199:VAL:HG13	1:F:200:VAL:N	2.36	0.41
1:F:206:TYR:CG	1:F:207:LEU:N	2.88	0.41
1:B:304:PHE:O	1:B:307:GLU:HB2	2.21	0.41
1:C:51:VAL:HG11	1:C:54:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:GLY:HA3	1:C:296:PHE:O	2.20	0.41
1:C:303:ALA:O	1:C:306:THR:HG23	2.20	0.41
1:D:199:VAL:HG13	1:D:200:VAL:N	2.35	0.41
1:E:214:VAL:O	1:E:214:VAL:HG12	2.20	0.41
1:A:199:VAL:HG13	1:A:200:VAL:N	2.35	0.41
1:B:188:ILE:HD11	1:B:263:MSE:CE	2.33	0.41
1:B:206:TYR:CG	1:B:207:LEU:N	2.89	0.41
1:C:199:VAL:HG13	1:C:311:PHE:CE2	2.48	0.41
1:C:234:ASP:HB3	1:C:237:VAL:HG23	2.03	0.41
1:E:199:VAL:CG1	1:E:311:PHE:HE2	2.29	0.41
1:E:206:TYR:CG	1:E:207:LEU:N	2.89	0.41
1:F:164:ILE:CD1	1:F:165:GLN:N	2.48	0.41
1:F:199:VAL:HG13	1:F:311:PHE:CE2	2.48	0.41
1:F:240:LYS:O	1:F:244:THR:CG2	2.67	0.41
1:B:303:ALA:O	1:B:306:THR:HG23	2.21	0.41
1:C:108:HIS:HE1	1:D:104:ASN:OD1	2.04	0.41
1:C:234:ASP:HB3	1:C:237:VAL:CG2	2.51	0.41
1:C:298:HIS:CD2	2:C:1318:DEP:H31	2.56	0.41
1:D:43:THR:HG23	1:D:60:THR:HB	1.89	0.41
1:E:83:PRO:HG3	1:E:317:LEU:HD23	2.02	0.41
1:E:138:MSE:HB2	1:E:224:GLU:OE1	2.21	0.41
1:F:139:THR:HG21	1:F:228:TYR:HB2	2.02	0.41
1:A:105:TRP:HB2	1:A:112:THR:HG21	2.02	0.40
1:A:181:SER:HA	1:A:204:TYR:O	2.21	0.40
1:D:177:VAL:CG1	1:D:200:VAL:HG22	2.52	0.40
1:D:199:VAL:CG1	1:D:311:PHE:HE2	2.30	0.40
1:E:139:THR:HG21	1:E:228:TYR:HB2	2.02	0.40
1:F:264:ALA:HB2	1:F:304:PHE:CE1	2.56	0.40
1:A:266:GLY:HA3	1:A:296:PHE:O	2.21	0.40
1:B:83:PRO:HG3	1:B:317:LEU:HD23	2.02	0.40
1:B:229:PHE:CE2	1:B:238:GLU:HA	2.57	0.40
1:C:69:ILE:HA	1:C:123:SER:HB3	2.03	0.40
1:A:58:ARG:HE	1:A:70:GLU:HG2	1.86	0.40
1:B:19:THR:O	1:B:20:ALA:C	2.59	0.40
1:D:206:TYR:CG	1:D:207:LEU:N	2.89	0.40
1:E:258:LYS:HD3	1:E:258:LYS:HA	1.76	0.40
1:F:38:VAL:O	1:F:159:ARG:NH1	2.44	0.40
1:E:78:GLN:O	1:E:82:HIS:HE1	2.03	0.40
1:F:177:VAL:CG1	1:F:200:VAL:HG22	2.52	0.40
1:B:15:LYS:O	1:B:16:PRO:C	2.59	0.40
1:B:15:LYS:O	1:B:16:PRO:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:THR:OG1	1:E:287:ASP:N	2.53	0.40
1:F:221:PRO:C	1:F:223:LEU:N	2.75	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	309/320 (97%)	296 (96%)	12 (4%)	1 (0%)	41	66
1	B	309/320 (97%)	292 (94%)	15 (5%)	2 (1%)	25	50
1	C	309/320 (97%)	297 (96%)	11 (4%)	1 (0%)	41	66
1	D	309/320 (97%)	298 (96%)	9 (3%)	2 (1%)	25	50
1	E	310/320 (97%)	298 (96%)	10 (3%)	2 (1%)	25	50
1	F	310/320 (97%)	295 (95%)	14 (4%)	1 (0%)	41	66
All	All	1856/1920 (97%)	1776 (96%)	71 (4%)	9 (0%)	29	54

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	PHE
1	D	122	GLY
1	E	64	PHE
1	F	122	GLY
1	C	122	GLY
1	A	122	GLY
1	B	16	PRO
1	E	122	GLY
1	B	204	TYR

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	246/266 (92%)	230 (94%)	16 (6%)	17	38
1	B	242/266 (91%)	220 (91%)	22 (9%)	9	21
1	C	242/266 (91%)	223 (92%)	19 (8%)	12	28
1	D	240/266 (90%)	224 (93%)	16 (7%)	16	37
1	E	247/266 (93%)	232 (94%)	15 (6%)	18	41
1	F	245/266 (92%)	227 (93%)	18 (7%)	14	33
All	All	1462/1596 (92%)	1356 (93%)	106 (7%)	14	33

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	35	LEU
1	A	37	GLN
1	A	41	GLU
1	A	70	GLU
1	A	112	THR
1	A	145	LYS
1	A	153	VAL
1	A	169	GLU
1	A	199	VAL
1	A	203	ASP
1	A	204	TYR
1	A	244	THR
1	A	261	THR
1	A	265	ILE
1	A	306	THR
1	B	7	SER
1	B	8	LEU
1	B	18	LYS
1	B	29	LYS
1	B	35	LEU
1	B	37	GLN

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Mol	Chain	Res	Type
1	B	43	THR
1	B	67	SER
1	B	112	THR
1	B	120	GLN
1	B	145	LYS
1	B	153	VAL
1	B	169	GLU
1	B	199	VAL
1	B	203	ASP
1	B	212	ARG
1	B	218	LEU
1	B	219	GLU
1	B	244	THR
1	B	261	THR
1	B	265	ILE
1	B	306	THR
1	C	21	ARG
1	C	35	LEU
1	C	37	GLN
1	C	41	GLU
1	C	43	THR
1	C	51	VAL
1	C	67	SER
1	C	112	THR
1	C	120	GLN
1	C	145	LYS
1	C	153	VAL
1	C	169	GLU
1	C	199	VAL
1	C	203	ASP
1	C	244	THR
1	C	261	THR
1	C	265	ILE
1	C	288	LYS
1	C	306	THR
1	D	21	ARG
1	D	35	LEU
1	D	37	GLN
1	D	79	THR
1	D	112	THR
1	D	145	LYS
1	D	153	VAL

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Mol	Chain	Res	Type
1	D	164	ILE
1	D	169	GLU
1	D	203	ASP
1	D	244	THR
1	D	261	THR
1	D	265	ILE
1	D	286	THR
1	D	290	LEU
1	D	306	THR
1	E	21	ARG
1	E	35	LEU
1	E	37	GLN
1	E	67	SER
1	E	112	THR
1	E	145	LYS
1	E	153	VAL
1	E	169	GLU
1	E	199	VAL
1	E	203	ASP
1	E	204	TYR
1	E	244	THR
1	E	261	THR
1	E	265	ILE
1	E	306	THR
1	F	7	SER
1	F	21	ARG
1	F	35	LEU
1	F	37	GLN
1	F	67	SER
1	F	68	LYS
1	F	112	THR
1	F	124	GLU
1	F	126	THR
1	F	145	LYS
1	F	153	VAL
1	F	169	GLU
1	F	203	ASP
1	F	204	TYR
1	F	244	THR
1	F	261	THR
1	F	265	ILE
1	F	306	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	108	HIS
1	A	133	HIS
1	A	173	HIS
1	A	220	GLN
1	A	232	ASN
1	A	305	GLN
1	B	62	GLN
1	B	82	HIS
1	B	89	HIS
1	B	108	HIS
1	B	133	HIS
1	B	220	GLN
1	C	82	HIS
1	C	89	HIS
1	C	133	HIS
1	C	220	GLN
1	C	232	ASN
1	D	82	HIS
1	D	89	HIS
1	D	108	HIS
1	D	133	HIS
1	D	220	GLN
1	D	232	ASN
1	E	62	GLN
1	E	78	GLN
1	E	89	HIS
1	E	133	HIS
1	E	220	GLN
1	E	232	ASN
1	F	78	GLN
1	F	89	HIS
1	F	133	HIS
1	F	220	GLN
1	F	232	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 (i)

6 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	DEP	B	1318	1	4,7,7	0.69	0	2,7,7	0.09	0
2	DEP	F	1319	1	4,7,7	0.70	0	2,7,7	0.10	0
2	DEP	A	1318	1	4,7,7	0.64	0	2,7,7	0.07	0
2	DEP	C	1318	1	4,7,7	0.69	0	2,7,7	0.08	0
2	DEP	E	1319	1	4,7,7	0.67	0	2,7,7	0.08	0
2	DEP	D	1318	1	4,7,7	0.67	0	2,7,7	0.07	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	DEP	B	1318	1	-	1/2/6/6	-
2	DEP	F	1319	1	-	0/2/6/6	-
2	DEP	A	1318	1	-	1/2/6/6	-
2	DEP	C	1318	1	-	1/2/6/6	-
2	DEP	E	1319	1	-	1/2/6/6	-
2	DEP	D	1318	1	-	0/2/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1318	DEP	C2-C1-O1-P
2	B	1318	DEP	C4-C3-O2-P
2	C	1318	DEP	C2-C1-O1-P
2	E	1319	DEP	C2-C1-O1-P

There are no ring outliers.

6 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1318	DEP	17	0
2	F	1319	DEP	17	0
2	A	1318	DEP	20	0
2	C	1318	DEP	17	0
2	E	1319	DEP	14	0
2	D	1318	DEP	10	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	308/320 (96%)	-0.24	0 100 100	30, 37, 47, 57	0
1	B	308/320 (96%)	-0.25	1 (0%) 94 95	29, 38, 50, 58	0
1	C	308/320 (96%)	-0.18	0 100 100	30, 42, 61, 89	0
1	D	308/320 (96%)	-0.09	1 (0%) 94 95	34, 46, 62, 69	0
1	E	309/320 (96%)	-0.18	1 (0%) 94 95	26, 38, 53, 67	0
1	F	309/320 (96%)	-0.17	1 (0%) 94 95	27, 37, 54, 69	0
All	All	1850/1920 (96%)	-0.18	4 (0%) 95 96	26, 40, 59, 89	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	126	THR	2.5
1	B	164	ILE	2.2
1	F	79	THR	2.2
1	D	157	ALA	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)

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(Å^2)	Q<0.9
2	DEP	F	1319	8/8	0.78	0.34	55,56,56,56	0
2	DEP	D	1318	8/8	0.81	0.26	69,69,70,70	0
2	DEP	B	1318	8/8	0.86	0.29	50,50,51,51	0
2	DEP	C	1318	8/8	0.88	0.23	59,59,59,59	0
2	DEP	E	1319	8/8	0.92	0.17	53,53,53,54	0
2	DEP	A	1318	8/8	0.93	0.17	57,58,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.