



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 11:47 AM EDT

PDB ID : 3HWS
Title : Crystal structure of nucleotide-bound hexameric ClpX
Authors : Glynn, S.E.; Martin, A.; Baker, T.A.; Sauer, R.T.
Deposited on : unknown
Resolution : 3.25 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

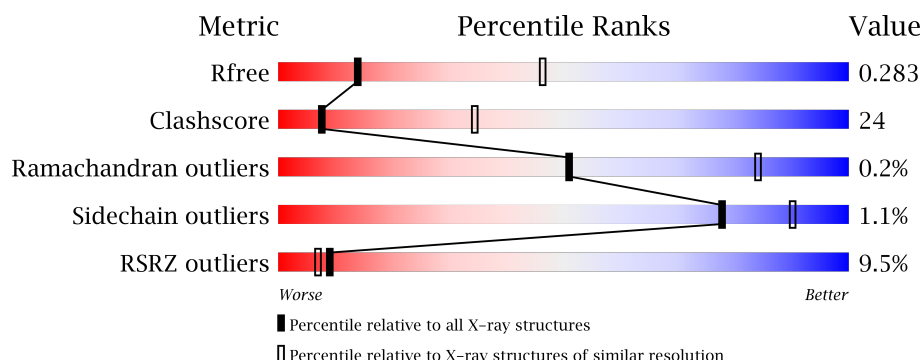
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>8%</div> <div>54%</div> <div>33%</div> <div>12%</div> </div>
1	B	363	<div> <div>7%</div> <div>54%</div> <div>32%</div> <div>13%</div> </div>
1	C	363	<div> <div>6%</div> <div>53%</div> <div>30%</div> <div>15%</div> </div>
1	D	363	<div> <div>10%</div> <div>52%</div> <div>35%</div> <div>13%</div> </div>
1	E	363	<div> <div>9%</div> <div>50%</div> <div>35%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	363	

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	ADP	D	602	-	-	-	X
2	ADP	E	603	-	-	X	-
3	SO4	B	702	-	-	-	X
3	SO4	D	710	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14292 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 ATP-dependent Clp protease ATP-binding subunit clpX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2381	1514	396	465	6			
1	B	315	Total	C	N	O	S	0	0	0
			2388	1519	405	458	6			
1	C	307	Total	C	N	O	S	0	0	0
			2333	1485	392	450	6			
1	D	316	Total	C	N	O	S	0	0	0
			2333	1485	393	449	6			
1	E	313	Total	C	N	O	S	0	0	0
			2310	1468	384	452	6			
1	F	314	Total	C	N	O	S	0	0	0
			2367	1502	398	461	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLN	GLU	ENGINEERED	UNP P0A6H1
A	408	GLU	LYS	ENGINEERED	UNP P0A6H1
B	185	GLN	GLU	ENGINEERED	UNP P0A6H1
B	408	GLU	LYS	ENGINEERED	UNP P0A6H1
C	185	GLN	GLU	ENGINEERED	UNP P0A6H1
C	408	GLU	LYS	ENGINEERED	UNP P0A6H1
D	185	GLN	GLU	ENGINEERED	UNP P0A6H1
D	408	GLU	LYS	ENGINEERED	UNP P0A6H1
E	185	GLN	GLU	ENGINEERED	UNP P0A6H1
E	408	GLU	LYS	ENGINEERED	UNP P0A6H1
F	185	GLN	GLU	ENGINEERED	UNP P0A6H1
F	408	GLU	LYS	ENGINEERED	UNP P0A6H1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	1	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	2	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	3	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	1	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

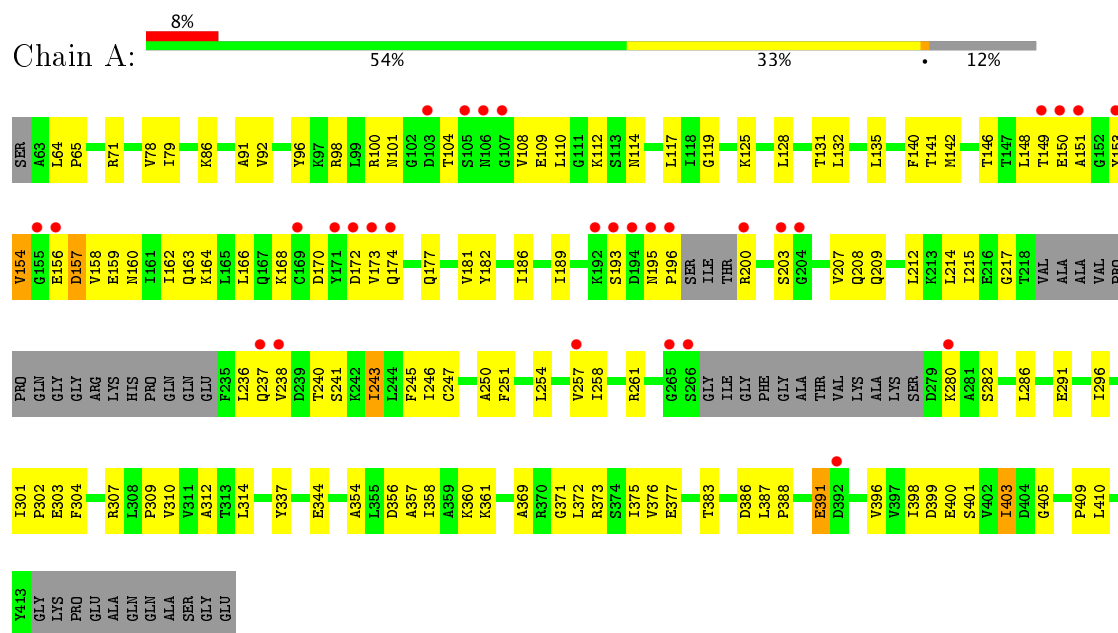
- Molecule 5 is water.

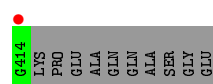
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0
5	C	3	Total O 3 3	0	0
5	E	1	Total O 1 1	0	0

3 Residue-property plots

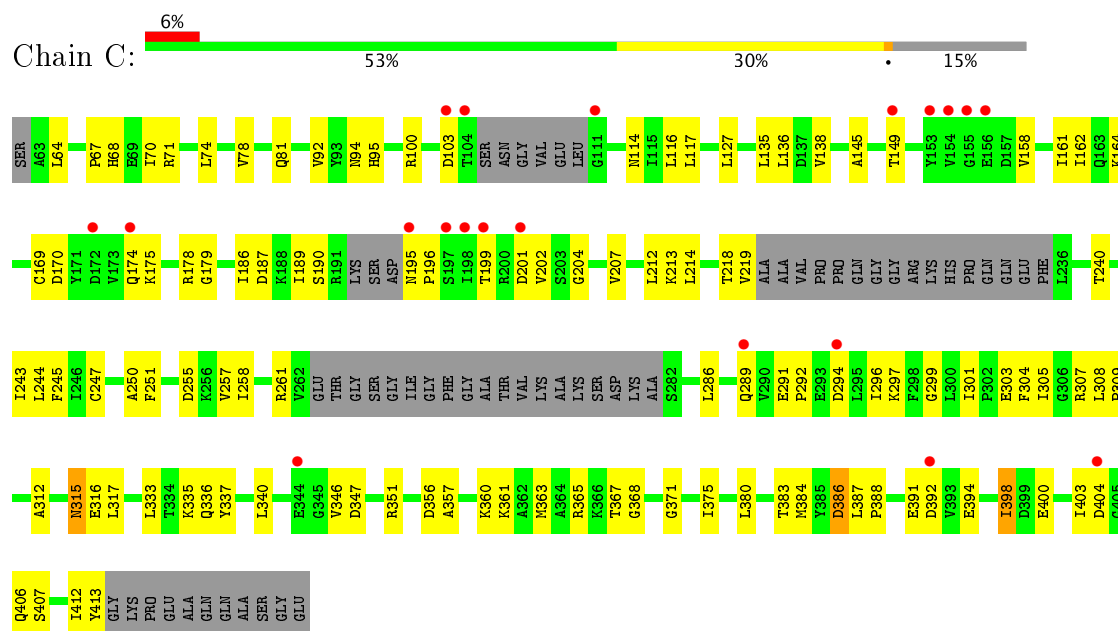
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ATP-dependent Clp protease ATP-binding subunit clpX

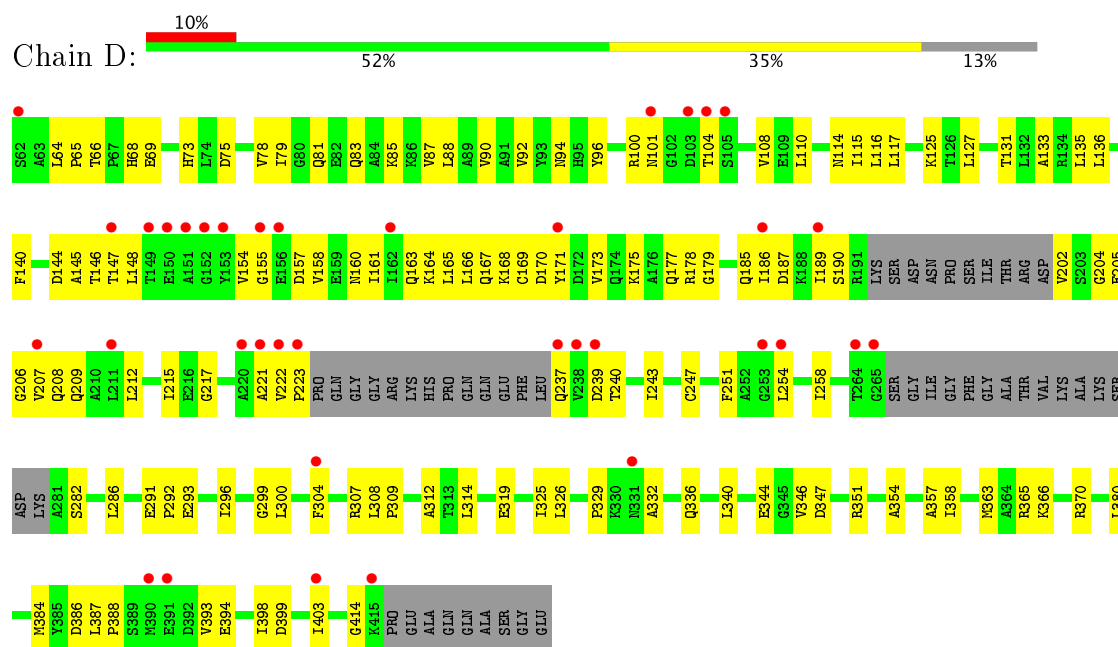




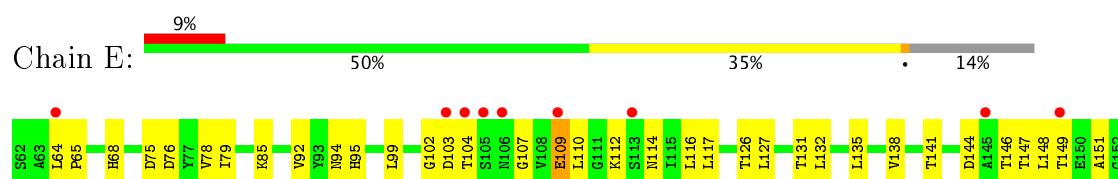
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX

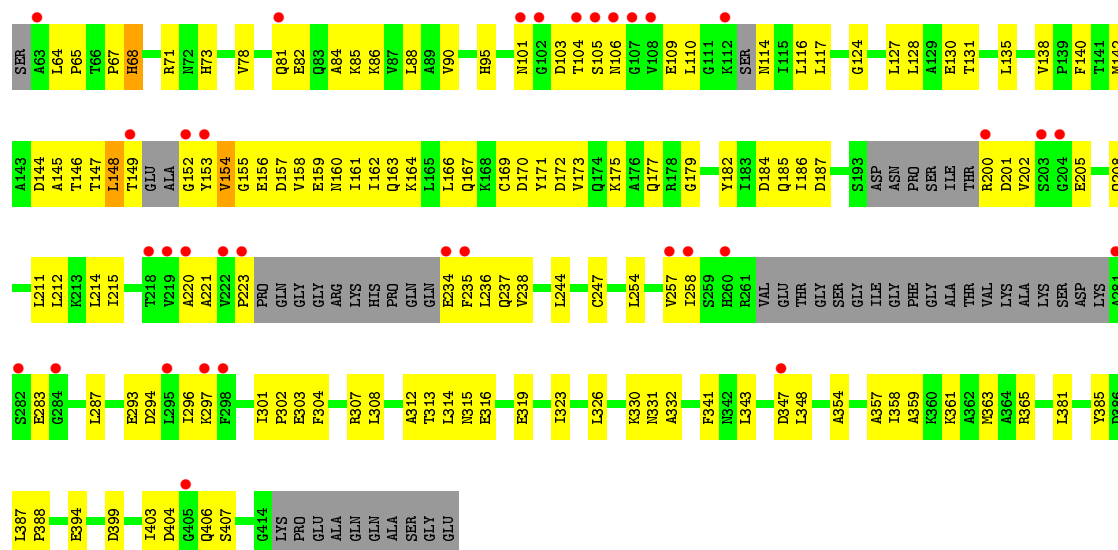


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX



- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.09Å 178.50Å 201.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.08 – 3.25 45.08 – 3.22	Depositor EDS
% Data completeness (in resolution range)	96.2 (45.08-3.25) 98.7 (45.08-3.22)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.282 0.238 , 0.283	Depositor DCC
R_{free} test set	1556 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 95.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14292	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, ADP

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	0.23	0/2408	0.41	0/3265
1	B	0.22	0/2416	0.39	0/3268
1	C	0.22	0/2359	0.39	0/3193
1	D	0.22	0/2360	0.39	0/3201
1	E	0.25	0/2337	0.44	0/3172
1	F	0.24	0/2393	0.40	0/3239
All	All	0.23	0/14273	0.41	0/19338

There are no bond length outliers.

There are no bond angle outliers.

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	2381	0	2363	115	0
1	B	2388	0	2417	104	0
1	C	2333	0	2370	105	0
1	D	2333	0	2317	118	0
1	E	2310	0	2279	170	0
1	F	2367	0	2362	125	0
2	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	3	0
2	D	27	0	12	4	0
2	E	27	0	12	9	0
3	A	15	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	1	0
5	E	1	0	0	0	0
All	All	14292	0	14156	693	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 24.

All (693) 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:E:147:THR:HG21	1:F:301:ILE:HG22	1.35	1.09
1:D:148:LEU:HD21	1:D:158:VAL:HG12	1.34	1.08
1:E:303:GLU:HG2	1:E:307:ARG:HH22	1.13	1.08
1:B:161:ILE:HA	1:B:164:LYS:HE2	1.35	1.07
1:A:150:GLU:HA	1:A:203:SER:CB	1.87	1.05
1:A:150:GLU:CA	1:A:203:SER:HB2	1.88	1.02
1:A:154:VAL:HA	1:A:157:ASP:HB3	1.41	1.01
1:A:151:ALA:HB3	1:A:154:VAL:HB	1.45	0.98
1:E:148:LEU:HA	1:E:154:VAL:HG21	1.41	0.98
1:E:177:GLN:HB3	1:E:238:VAL:HG21	1.45	0.98
1:F:152:GLY:O	1:F:154:VAL:HG23	1.64	0.97
1:A:150:GLU:HA	1:A:203:SER:HB2	0.99	0.96
1:B:186:ILE:HG13	1:B:247:CYS:HB3	1.49	0.92
1:D:186:ILE:HG13	1:D:247:CYS:HB3	1.52	0.92
1:B:229:LYS:HD2	1:B:233:GLN:HB3	1.52	0.91
1:F:158:VAL:HB	1:F:214:LEU:HD23	1.53	0.91
1:B:148:LEU:HB3	1:B:154:VAL:HG23	1.54	0.90
1:E:212:LEU:HD22	1:E:307:ARG:HH21	1.37	0.89
1:E:173:VAL:HG13	1:E:238:VAL:HB	1.54	0.89
1:E:151:ALA:O	1:E:154:VAL:HG12	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASP:O	1:D:147:THR:HG22	1.74	0.87
1:A:186:ILE:HG13	1:A:247:CYS:HB3	1.58	0.85
1:C:169:CYS:SG	1:C:175:LYS:HB2	2.17	0.85
1:A:148:LEU:O	1:A:154:VAL:HG11	1.77	0.85
1:E:154:VAL:O	1:E:158:VAL:HG23	1.76	0.83
1:A:357:ALA:HB1	1:A:403:ILE:HG23	1.58	0.83
1:D:155:GLY:O	1:D:158:VAL:HG22	1.78	0.83
1:E:148:LEU:CA	1:E:154:VAL:HG21	2.08	0.83
1:A:148:LEU:HA	1:A:154:VAL:HG21	1.61	0.83
1:A:280:LYS:CB	1:A:286:LEU:HD11	2.09	0.82
1:F:81:GLN:HE22	1:F:316:GLU:H	1.26	0.81
1:A:215:ILE:HG21	1:A:307:ARG:HB3	1.61	0.81
1:E:357:ALA:HB1	1:E:403:ILE:HG23	1.62	0.80
1:F:173:VAL:HG13	1:F:238:VAL:HG22	1.62	0.80
1:C:186:ILE:HG13	1:C:247:CYS:HB3	1.61	0.79
1:F:71:ARG:HG3	1:F:85:LYS:HB3	1.65	0.78
1:A:337:TYR:OH	1:A:377:GLU:HG2	1.82	0.78
1:E:144:ASP:O	1:E:148:LEU:HG	1.84	0.78
1:E:147:THR:CG2	1:F:301:ILE:HG22	2.14	0.77
1:A:114:ASN:ND2	1:A:215:ILE:HG23	2.01	0.76
1:E:157:ASP:O	1:E:160:ASN:HB3	1.85	0.76
1:C:315:ASN:H	1:C:315:ASN:HD22	1.31	0.75
1:E:157:ASP:OD1	1:E:157:ASP:C	2.23	0.75
1:E:127:LEU:HD22	2:E:603:ADP:H2'	1.67	0.75
1:A:157:ASP:O	1:A:160:ASN:HB3	1.86	0.75
1:A:149:THR:HA	1:A:207:VAL:HG21	1.68	0.75
1:E:303:GLU:HG2	1:E:307:ARG:NH2	1.98	0.75
1:B:169:CYS:SG	1:B:175:LYS:HB2	2.26	0.75
1:A:214:LEU:HD22	1:A:240:THR:HG21	1.68	0.74
1:E:156:GLU:O	1:E:159:GLU:HG2	1.87	0.74
1:B:64:LEU:HD12	1:B:65:PRO:HD2	1.67	0.74
1:D:64:LEU:HD12	1:D:65:PRO:HD2	1.69	0.73
1:E:64:LEU:HD12	1:E:65:PRO:HD2	1.69	0.73
1:D:217:GLY:HA2	1:D:240:THR:OG1	1.88	0.73
1:A:399:ASP:O	1:A:403:ILE:HG12	1.89	0.73
1:B:229:LYS:HD2	1:B:233:GLN:CB	2.19	0.72
1:F:144:ASP:OD1	1:F:185:GLN:HG3	1.89	0.72
1:D:357:ALA:HB1	1:D:403:ILE:HG12	1.72	0.72
1:A:373:ARG:HD3	1:B:309:PRO:HB3	1.72	0.72
1:C:175:LYS:HD3	1:C:178:ARG:HH12	1.51	0.72
1:D:189:ILE:HD11	1:D:204:GLY:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LYS:O	1:D:167:GLN:HG2	1.89	0.71
1:E:236:LEU:HD23	1:E:236:LEU:H	1.55	0.71
1:B:164:LYS:HG2	1:C:213:LYS:HD2	1.73	0.71
1:E:148:LEU:O	1:E:154:VAL:HG11	1.91	0.71
1:F:81:GLN:NE2	1:F:316:GLU:H	1.88	0.70
1:F:158:VAL:HB	1:F:214:LEU:CD2	2.21	0.70
1:F:211:LEU:O	1:F:214:LEU:HG	1.90	0.70
1:B:233:GLN:CD	1:B:234:GLU:H	1.94	0.70
1:D:64:LEU:HB2	1:D:100:ARG:HH11	1.55	0.70
1:A:173:VAL:HG13	1:A:238:VAL:HG22	1.74	0.70
1:F:114:ASN:HB3	1:F:308:LEU:HD13	1.74	0.70
1:B:230:HIS:N	1:B:231:PRO:HD2	2.07	0.69
1:E:399:ASP:O	1:E:403:ILE:HG12	1.92	0.69
1:D:144:ASP:HB3	1:D:147:THR:HG22	1.73	0.69
1:F:162:ILE:O	1:F:166:LEU:HD12	1.92	0.69
1:B:212:LEU:CD1	1:B:304:PHE:HA	2.22	0.69
1:B:158:VAL:HG13	1:B:214:LEU:HD22	1.74	0.69
1:C:186:ILE:O	1:C:189:ILE:HG12	1.93	0.69
1:D:169:CYS:SG	1:D:175:LYS:HB2	2.32	0.69
1:B:205:GLU:HA	1:B:208:GLN:HG3	1.74	0.69
1:A:112:LYS:HE3	1:A:307:ARG:HE	1.56	0.68
1:B:160:ASN:O	1:B:164:LYS:HG3	1.93	0.68
1:B:150:GLU:O	1:C:196:PRO:HG3	1.92	0.68
1:A:151:ALA:HB2	1:A:153:TYR:CZ	2.29	0.68
1:A:212:LEU:CD1	1:A:307:ARG:HG3	2.22	0.68
1:B:211:LEU:O	1:B:215:ILE:HG12	1.93	0.68
1:A:149:THR:HA	1:A:207:VAL:CG2	2.24	0.68
1:D:66:THR:HG23	1:D:69:GLU:H	1.58	0.68
1:F:236:LEU:H	1:F:236:LEU:HD23	1.58	0.68
1:B:365:ARG:HG3	1:B:367:THR:HG23	1.76	0.68
1:B:212:LEU:HD11	1:B:303:GLU:O	1.93	0.67
1:C:158:VAL:HG11	1:C:214:LEU:HB2	1.75	0.67
1:C:400:GLU:HB2	1:C:406:GLN:HE21	1.59	0.67
1:B:138:VAL:HG13	1:B:179:GLY:HA2	1.77	0.67
1:A:217:GLY:HA2	1:A:240:THR:OG1	1.95	0.67
1:D:131:THR:O	1:D:135:LEU:HG	1.94	0.67
1:B:149:THR:HA	1:B:207:VAL:HG21	1.76	0.67
1:D:116:LEU:HB2	1:D:308:LEU:HD23	1.75	0.67
1:A:243:ILE:HD11	1:A:245:PHE:CZ	2.29	0.67
1:A:212:LEU:HD11	1:A:307:ARG:HG3	1.77	0.67
1:E:388:PRO:HG2	1:F:67:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ILE:HD11	1:C:214:LEU:HD22	1.76	0.66
1:A:282:SER:O	1:A:286:LEU:HD13	1.95	0.66
1:B:327:LYS:O	1:B:335:LYS:HE3	1.95	0.66
1:D:291:GLU:HG3	1:D:292:PRO:HD2	1.77	0.66
1:F:81:GLN:HE22	1:F:315:ASN:N	1.94	0.66
1:B:177:GLN:HG3	1:B:238:VAL:HG23	1.78	0.65
1:B:141:THR:HG22	1:B:165:LEU:HD13	1.78	0.65
1:F:399:ASP:O	1:F:403:ILE:HG12	1.96	0.65
1:F:357:ALA:HB1	1:F:403:ILE:HG23	1.79	0.65
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.79	0.65
1:D:64:LEU:HB2	1:D:100:ARG:NH1	2.11	0.65
1:C:81:GLN:HE22	1:C:316:GLU:H	1.44	0.65
1:E:104:THR:HG21	1:E:109:GLU:N	2.11	0.65
1:C:158:VAL:O	1:C:161:ILE:HG12	1.97	0.65
1:E:104:THR:CG2	1:E:109:GLU:HB2	2.27	0.65
1:E:367:THR:HG21	1:E:371:GLY:HA3	1.79	0.65
1:E:370:ARG:HG2	2:E:603:ADP:H5'2	1.79	0.65
1:E:169:CYS:SG	1:E:176:ALA:HB2	2.37	0.65
1:A:117:LEU:HD23	1:A:312:ALA:HB3	1.78	0.64
1:E:149:THR:HA	1:E:207:VAL:HG11	1.78	0.64
1:B:291:GLU:HB2	1:B:293:GLU:HG2	1.79	0.64
1:E:301:ILE:HG13	1:E:304:PHE:H	1.61	0.64
1:E:147:THR:HG21	1:F:301:ILE:CG2	2.21	0.64
1:A:146:THR:O	1:A:149:THR:HG22	1.98	0.64
1:B:385:TYR:OH	1:C:71:ARG:HD3	1.98	0.64
1:A:151:ALA:O	1:A:154:VAL:HG12	1.97	0.63
1:C:367:THR:HB	1:D:291:GLU:HG2	1.78	0.63
1:F:211:LEU:O	1:F:215:ILE:HD12	1.98	0.63
1:C:392:ASP:HB2	1:C:412:ILE:O	1.98	0.63
1:C:335:LYS:HB3	1:D:108:VAL:HG11	1.79	0.63
1:C:138:VAL:HG12	1:C:179:GLY:HA2	1.81	0.63
1:E:212:LEU:HD21	1:E:304:PHE:HD1	1.63	0.63
1:E:212:LEU:HD22	1:E:307:ARG:NH2	2.11	0.63
1:E:92:VAL:HG21	1:E:132:LEU:HD13	1.79	0.63
1:E:212:LEU:CD2	1:E:307:ARG:HH21	2.11	0.63
1:C:357:ALA:O	1:C:361:LYS:HG2	1.99	0.62
1:E:258:ILE:HD11	1:E:290:VAL:HG23	1.81	0.62
1:E:303:GLU:CG	1:E:307:ARG:HH22	2.02	0.62
1:E:347:ASP:O	1:E:394:GLU:HG3	1.99	0.62
1:B:351:ARG:HD3	1:B:398:ILE:HG22	1.81	0.62
1:A:200:ARG:N	1:A:200:ARG:HD2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:O	1:B:189:ILE:HG12	2.00	0.62
1:E:159:GLU:HB2	1:E:235:PHE:CZ	2.35	0.62
1:A:148:LEU:HA	1:A:154:VAL:CG2	2.30	0.62
1:B:148:LEU:HB3	1:B:154:VAL:CG2	2.28	0.62
1:B:214:LEU:HD12	1:B:240:THR:HG21	1.81	0.62
1:E:403:ILE:HG13	1:E:404:ASP:H	1.65	0.62
1:D:365:ARG:O	1:D:366:LYS:HG2	2.00	0.62
1:C:162:ILE:HD11	1:C:214:LEU:HD11	1.81	0.62
1:E:104:THR:HG22	1:E:109:GLU:HB2	1.82	0.62
1:B:362:ALA:O	1:B:365:ARG:HG2	1.99	0.61
1:E:186:ILE:HD12	1:E:247:CYS:HB3	1.80	0.61
1:E:370:ARG:HG2	2:E:603:ADP:C5'	2.31	0.61
1:B:138:VAL:CG1	1:B:179:GLY:HA2	2.30	0.61
1:D:144:ASP:HB3	1:D:147:THR:CG2	2.30	0.61
1:F:211:LEU:HD12	1:F:214:LEU:HD21	1.82	0.61
1:D:386:ASP:HB3	1:E:68:HIS:NE2	2.15	0.61
1:F:403:ILE:HG13	1:F:404:ASP:N	2.16	0.61
1:C:212:LEU:HD11	1:C:307:ARG:HG3	1.83	0.61
1:B:212:LEU:HD13	1:B:304:PHE:HA	1.82	0.61
1:A:114:ASN:HD21	1:A:215:ILE:HG23	1.66	0.60
1:D:319:GLU:CD	1:D:319:GLU:H	2.04	0.60
1:F:147:THR:O	1:F:149:THR:HG23	2.01	0.60
1:B:340:LEU:HD21	1:C:94:ASN:ND2	2.16	0.60
1:F:301:ILE:HG12	1:F:304:PHE:HB2	1.83	0.60
1:C:258:ILE:HD13	1:C:286:LEU:O	2.02	0.60
1:E:166:LEU:HA	1:E:169:CYS:SG	2.41	0.60
1:D:158:VAL:O	1:D:161:ILE:HG12	2.02	0.59
1:C:161:ILE:HA	1:C:164:LYS:HE2	1.83	0.59
1:B:190:SER:HB2	1:B:299:GLY:HA3	1.85	0.59
1:D:399:ASP:O	1:D:403:ILE:HG13	2.03	0.59
1:F:64:LEU:N	1:F:65:PRO:HD3	2.17	0.59
1:E:296:ILE:CD1	1:E:305:ILE:HD12	2.32	0.59
1:F:173:VAL:O	1:F:177:GLN:HG3	2.03	0.59
1:D:81:GLN:O	1:D:85:LYS:HG3	2.02	0.59
1:A:156:GLU:O	1:A:159:GLU:HG2	2.02	0.59
1:E:151:ALA:HB3	1:E:154:VAL:HB	1.86	0.58
1:B:76:ASP:O	1:B:329:PRO:HA	2.03	0.58
1:D:177:GLN:OE1	1:D:239:ASP:HB2	2.04	0.58
1:B:259:SER:OG	1:B:286:LEU:HD21	2.04	0.58
1:D:293:GLU:HA	1:D:296:ILE:HG22	1.85	0.58
1:A:200:ARG:HD3	1:B:191:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLY:HA2	1:B:240:THR:OG1	2.04	0.58
1:B:117:LEU:HD23	1:B:312:ALA:HB3	1.85	0.58
1:E:212:LEU:HD21	1:E:304:PHE:HA	1.85	0.58
1:E:211:LEU:O	1:E:215:ILE:HG13	2.03	0.58
1:E:292:PRO:O	1:E:296:ILE:HG12	2.03	0.58
1:E:212:LEU:HD13	1:E:307:ARG:NH2	2.19	0.58
1:A:154:VAL:O	1:A:158:VAL:HG23	2.03	0.58
1:C:175:LYS:HD3	1:C:178:ARG:NH1	2.18	0.58
1:F:73:HIS:CD2	1:F:135:LEU:HD13	2.38	0.58
1:E:213:LYS:HG2	1:E:214:LEU:N	2.19	0.57
1:F:186:ILE:HG21	1:F:247:CYS:HB3	1.85	0.57
1:E:79:ILE:H	2:E:603:ADP:HN62	1.52	0.57
1:A:71:ARG:HD3	1:F:385:TYR:OH	2.04	0.57
1:B:205:GLU:O	1:B:208:GLN:HB2	2.05	0.57
1:C:158:VAL:CG1	1:C:214:LEU:HB2	2.33	0.57
1:D:75:ASP:HA	1:D:85:LYS:NZ	2.20	0.57
1:C:365:ARG:HB2	1:C:367:THR:HG23	1.86	0.57
1:E:104:THR:HG21	1:E:110:LEU:N	2.19	0.57
1:F:138:VAL:HG13	1:F:179:GLY:HA2	1.86	0.57
1:A:356:ASP:O	1:A:360:LYS:HG3	2.05	0.57
1:C:212:LEU:HD21	1:C:303:GLU:HG2	1.86	0.57
1:E:398:ILE:HD12	1:E:401:SER:H	1.69	0.57
1:A:157:ASP:C	1:A:157:ASP:OD1	2.43	0.56
1:E:126:THR:HG22	1:E:182:TYR:CE2	2.39	0.56
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.87	0.56
1:E:153:TYR:HB3	1:F:202:VAL:HG11	1.85	0.56
1:D:370:ARG:CG	2:D:602:ADP:H5'1	2.35	0.56
1:C:292:PRO:O	1:C:296:ILE:HG13	2.06	0.56
1:E:210:ALA:HA	1:E:213:LYS:HD3	1.86	0.56
1:A:212:LEU:HD21	1:A:303:GLU:CG	2.35	0.56
1:D:114:ASN:HD21	1:D:215:ILE:HG23	1.69	0.56
1:E:186:ILE:O	1:E:189:ILE:HG12	2.05	0.56
1:E:209:GLN:HA	1:E:212:LEU:HD12	1.87	0.56
1:A:357:ALA:O	1:A:361:LYS:HG2	2.06	0.56
1:A:383:THR:OG1	1:A:409:PRO:HG3	2.06	0.56
1:E:367:THR:CG2	1:E:371:GLY:HA3	2.36	0.56
1:E:331:ASN:CG	1:F:109:GLU:HG2	2.26	0.56
1:F:130:GLU:HG2	1:F:140:PHE:CE2	2.41	0.56
1:F:146:THR:C	1:F:148:LEU:HD23	2.26	0.56
1:F:200:ARG:HG3	1:F:201:ASP:N	2.21	0.56
1:F:293:GLU:O	1:F:297:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ARG:HG2	2:D:602:ADP:H5'1	1.88	0.55
1:D:319:GLU:HG3	1:D:363:MET:SD	2.47	0.55
1:E:177:GLN:HA	1:E:243:ILE:HG22	1.88	0.55
1:C:189:ILE:O	1:C:204:GLY:HA3	2.06	0.55
1:F:301:ILE:HG13	1:F:304:PHE:H	1.71	0.55
1:A:154:VAL:CA	1:A:157:ASP:HB3	2.25	0.55
1:E:189:ILE:HB	1:E:207:VAL:HG21	1.89	0.55
1:D:254:LEU:O	1:D:258:ILE:HG13	2.06	0.55
1:E:210:ALA:O	1:E:213:LYS:HG2	2.07	0.55
1:C:95:HIS:CD2	1:C:244:LEU:HD13	2.42	0.55
1:C:258:ILE:HD11	1:C:289:GLN:C	2.27	0.55
1:D:251:PHE:HB3	1:D:254:LEU:HB2	1.89	0.55
1:F:114:ASN:HD21	1:F:215:ILE:HG21	1.71	0.55
1:D:215:ILE:HG21	1:D:307:ARG:HB3	1.89	0.54
1:B:98:ARG:HG3	1:B:110:LEU:HD12	1.89	0.54
1:E:322:LEU:HD23	1:E:372:LEU:HD21	1.89	0.54
1:D:92:VAL:HG11	1:D:136:LEU:HD11	1.89	0.54
1:D:160:ASN:O	1:D:164:LYS:HG3	2.07	0.54
1:A:307:ARG:O	1:A:309:PRO:HD3	2.07	0.54
1:B:392:ASP:OD2	1:B:411:LEU:HG	2.07	0.54
1:D:148:LEU:HD21	1:D:158:VAL:CG1	2.23	0.54
1:F:387:LEU:HB3	1:F:388:PRO:HD3	1.89	0.54
1:A:151:ALA:HB1	1:A:153:TYR:CD1	2.42	0.54
1:B:307:ARG:C	1:B:309:PRO:HD3	2.28	0.54
1:B:386:ASP:HA	1:C:68:HIS:CD2	2.43	0.54
1:E:243:ILE:HD11	1:E:245:PHE:CZ	2.43	0.54
1:F:138:VAL:CG1	1:F:179:GLY:HA2	2.37	0.54
1:A:98:ARG:HD2	1:A:110:LEU:CB	2.38	0.53
1:A:344:GLU:HG3	1:A:387:LEU:HD21	1.89	0.53
1:D:351:ARG:HG3	1:D:398:ILE:HG22	1.90	0.53
1:E:148:LEU:HA	1:E:154:VAL:CG2	2.28	0.53
1:E:254:LEU:O	1:E:258:ILE:HG12	2.08	0.53
1:E:235:PHE:CE1	1:E:236:LEU:HD22	2.44	0.53
1:B:208:GLN:OE1	1:B:301:ILE:HG23	2.09	0.53
1:F:169:CYS:SG	1:F:175:LYS:HB2	2.48	0.53
1:C:392:ASP:HB3	1:C:413:TYR:CD2	2.43	0.53
1:E:358:ILE:HD13	1:E:376:VAL:HG22	1.90	0.53
1:A:140:PHE:CE2	1:A:142:MET:HG3	2.44	0.53
1:E:104:THR:HG21	1:E:109:GLU:H	1.72	0.53
1:F:145:ALA:HB3	1:F:185:GLN:HB2	1.90	0.53
1:F:220:ALA:HA	1:F:237:GLN:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:CB	1:A:108:VAL:HB	2.40	0.52
1:A:154:VAL:O	1:A:158:VAL:N	2.42	0.52
1:A:172:ASP:OD1	1:A:174:GLN:HG2	2.09	0.52
1:D:144:ASP:OD2	1:D:146:THR:OG1	2.27	0.52
1:E:104:THR:HG21	1:E:109:GLU:CA	2.38	0.52
1:E:331:ASN:OD1	1:F:109:GLU:HG2	2.09	0.52
1:F:116:LEU:HD12	1:F:247:CYS:O	2.09	0.52
1:D:354:ALA:O	1:D:358:ILE:HG13	2.10	0.52
1:A:212:LEU:HD21	1:A:303:GLU:HG3	1.92	0.52
1:E:104:THR:HG21	1:E:110:LEU:H	1.74	0.52
1:E:208:GLN:O	1:E:212:LEU:HG	2.10	0.52
1:F:234:GLU:HG2	1:F:235:PHE:CD2	2.44	0.52
1:C:161:ILE:HD11	1:C:214:LEU:CD2	2.39	0.52
1:A:109:GLU:HG3	1:F:330:LYS:O	2.10	0.52
1:E:95:HIS:NE2	1:E:99:LEU:HD11	2.24	0.52
1:A:254:LEU:O	1:A:257:VAL:HG12	2.10	0.52
1:B:154:VAL:HG21	1:B:207:VAL:HG22	1.91	0.52
1:C:255:ASP:O	1:C:258:ILE:HG22	2.10	0.52
1:B:386:ASP:HB3	1:C:68:HIS:NE2	2.25	0.52
1:D:145:ALA:HB3	1:D:185:GLN:O	2.08	0.52
1:D:293:GLU:O	1:D:296:ILE:HG22	2.09	0.52
1:A:358:ILE:HD13	1:A:376:VAL:HG22	1.91	0.52
1:B:232:GLN:O	1:B:233:GLN:HG3	2.09	0.52
1:C:406:GLN:HG3	1:C:407:SER:N	2.25	0.52
1:D:96:TYR:CE1	1:D:136:LEU:HD13	2.45	0.52
1:C:404:ASP:HB3	1:C:406:GLN:HG2	1.91	0.52
1:D:127:LEU:HD22	2:D:602:ADP:H2'	1.92	0.52
1:A:149:THR:CA	1:A:207:VAL:HG21	2.39	0.52
1:E:138:VAL:CG1	1:E:179:GLY:HA2	2.39	0.52
1:E:148:LEU:HB3	1:E:154:VAL:HG21	1.92	0.52
1:F:110:LEU:N	1:F:110:LEU:HD12	2.25	0.52
1:D:282:SER:O	1:D:286:LEU:HG	2.10	0.52
1:E:138:VAL:HG13	1:E:179:GLY:HA2	1.92	0.52
1:F:177:GLN:HG2	1:F:238:VAL:HG13	1.90	0.51
1:F:319:GLU:O	1:F:323:ILE:HG13	2.10	0.51
1:B:167:GLN:NE2	1:C:218:THR:HG22	2.25	0.51
1:C:291:GLU:CG	1:C:292:PRO:HD2	2.39	0.51
1:C:351:ARG:HG3	1:C:398:ILE:HG22	1.92	0.51
1:D:387:LEU:HB3	1:D:388:PRO:HD3	1.91	0.51
1:B:135:LEU:HD12	1:B:136:LEU:HG	1.91	0.51
1:E:388:PRO:HG2	1:F:67:PRO:CD	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:SER:O	1:A:196:PRO:HD3	2.10	0.51
1:E:403:ILE:HG13	1:E:404:ASP:N	2.23	0.51
1:A:91:ALA:HB2	1:A:310:VAL:HG11	1.91	0.51
1:D:205:GLU:O	1:D:208:GLN:HB2	2.11	0.51
1:D:344:GLU:OE2	1:D:388:PRO:HG3	2.11	0.51
1:E:79:ILE:N	2:E:603:ADP:HN62	2.08	0.51
1:E:144:ASP:OD2	1:F:302:PRO:HD3	2.11	0.51
1:E:325:ILE:HG23	2:E:603:ADP:N3	2.26	0.51
1:A:78:VAL:HG21	1:A:128:LEU:HD23	1.93	0.51
1:C:240:THR:O	1:C:243:ILE:HG12	2.10	0.51
1:E:148:LEU:CB	1:E:154:VAL:HG21	2.40	0.51
1:B:399:ASP:O	1:B:403:ILE:HG22	2.11	0.51
1:E:251:PHE:HB3	1:E:254:LEU:HB3	1.92	0.51
1:E:212:LEU:HD11	1:E:301:ILE:HD11	1.93	0.51
1:C:398:ILE:HG13	1:C:400:GLU:HG2	1.92	0.51
1:D:104:THR:HG22	1:D:110:LEU:HB3	1.92	0.51
1:E:212:LEU:CD2	1:E:304:PHE:HD1	2.22	0.51
1:F:144:ASP:O	1:F:147:THR:HG22	2.10	0.51
1:F:81:GLN:HE22	1:F:316:GLU:N	2.02	0.51
1:B:387:LEU:HB3	1:B:388:PRO:HD3	1.91	0.50
1:A:101:ASN:HD22	1:F:343:LEU:HD22	1.76	0.50
1:A:209:GLN:O	1:A:212:LEU:HB3	2.11	0.50
1:B:177:GLN:HB3	1:B:242:LYS:HB2	1.92	0.50
1:C:336:GLN:O	1:C:340:LEU:HD13	2.11	0.50
1:E:189:ILE:HD12	1:E:207:VAL:HG23	1.94	0.50
1:F:287:LEU:HD23	1:F:313:THR:HB	1.94	0.50
1:E:160:ASN:OD1	1:E:160:ASN:O	2.30	0.50
1:A:108:VAL:HG12	1:A:109:GLU:N	2.26	0.50
1:E:79:ILE:H	2:E:603:ADP:N6	2.09	0.50
1:F:186:ILE:HG13	1:F:187:ASP:N	2.25	0.50
1:F:152:GLY:O	1:F:154:VAL:CG2	2.49	0.50
1:C:307:ARG:O	1:C:309:PRO:HD3	2.12	0.50
1:D:296:ILE:HD12	1:D:300:LEU:O	2.12	0.50
1:E:258:ILE:O	1:E:262:VAL:HG22	2.11	0.50
1:F:403:ILE:HG13	1:F:404:ASP:H	1.75	0.50
1:E:99:LEU:HD13	1:E:242:LYS:HE3	1.93	0.50
1:F:155:GLY:O	1:F:158:VAL:HG22	2.11	0.50
1:D:187:ASP:OD1	1:D:187:ASP:N	2.45	0.49
1:A:391:GLU:N	1:A:391:GLU:CD	2.66	0.49
1:D:307:ARG:O	1:D:309:PRO:HD3	2.12	0.49
1:E:343:LEU:HD22	1:F:101:ASN:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ASN:O	1:F:164:LYS:HG3	2.12	0.49
1:A:96:TYR:O	1:A:100:ARG:HG3	2.12	0.49
1:E:293:GLU:H	1:E:293:GLU:CD	2.16	0.49
1:F:354:ALA:O	1:F:358:ILE:HG13	2.11	0.49
1:B:258:ILE:O	1:B:261:ARG:HG2	2.12	0.49
1:E:257:VAL:HA	1:E:260:HIS:HD2	1.77	0.49
1:A:148:LEU:O	1:A:154:VAL:HG21	2.13	0.49
1:A:141:THR:CG2	1:A:181:VAL:HG22	2.43	0.49
1:E:370:ARG:HD3	2:E:603:ADP:H4'	1.95	0.49
1:F:149:THR:C	1:F:157:ASP:CB	2.81	0.49
1:B:170:ASP:O	1:B:171:TYR:HB2	2.12	0.49
1:C:199:THR:HG22	1:C:201:ASP:H	1.78	0.49
1:D:96:TYR:O	1:D:100:ARG:HG3	2.12	0.49
1:D:307:ARG:C	1:D:309:PRO:HD3	2.33	0.49
1:F:236:LEU:CD2	1:F:236:LEU:H	2.26	0.49
1:A:119:GLY:O	1:A:250:ALA:HA	2.12	0.49
1:E:296:ILE:HD13	1:E:305:ILE:HD12	1.93	0.49
1:F:81:GLN:HE22	1:F:315:ASN:H	1.60	0.49
1:C:386:ASP:HB3	1:D:68:HIS:NE2	2.27	0.49
1:E:99:LEU:HD22	1:E:242:LYS:HG3	1.94	0.49
1:F:301:ILE:HG12	1:F:304:PHE:CB	2.43	0.49
1:C:315:ASN:HD22	1:C:315:ASN:N	2.03	0.48
1:D:64:LEU:CD1	1:D:65:PRO:HD2	2.42	0.48
1:E:208:GLN:OE1	1:E:301:ILE:HG12	2.12	0.48
1:F:301:ILE:CG1	1:F:304:PHE:HB2	2.42	0.48
1:A:109:GLU:HG3	1:F:331:ASN:HA	1.94	0.48
1:D:222:VAL:N	1:D:223:PRO:CD	2.76	0.48
1:E:177:GLN:HB2	1:E:242:LYS:HD3	1.96	0.48
1:F:153:TYR:O	1:F:154:VAL:HB	2.12	0.48
1:F:221:ALA:O	1:F:223:PRO:HD3	2.13	0.48
1:E:163:GLN:HA	1:E:166:LEU:HG	1.95	0.48
1:E:173:VAL:HG21	1:E:237:GLN:OE1	2.13	0.48
1:E:95:HIS:O	1:E:99:LEU:HG	2.13	0.48
1:F:202:VAL:HA	1:F:205:GLU:HG3	1.95	0.48
1:C:243:ILE:HD11	1:C:245:PHE:CZ	2.47	0.48
1:C:117:LEU:HD23	1:C:312:ALA:HB3	1.95	0.48
1:D:169:CYS:O	1:D:170:ASP:HB2	2.14	0.48
1:E:212:LEU:HD13	1:E:307:ARG:HH21	1.79	0.48
1:D:251:PHE:HB3	1:D:254:LEU:CB	2.44	0.48
1:D:164:LYS:NZ	1:E:209:GLN:HE22	2.10	0.48
1:F:254:LEU:O	1:F:258:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:O	1:A:237:GLN:HG2	2.14	0.48
1:A:243:ILE:HD11	1:A:245:PHE:CE2	2.49	0.48
1:C:403:ILE:HG23	1:C:404:ASP:N	2.29	0.48
1:D:157:ASP:OD1	1:D:157:ASP:C	2.52	0.48
1:D:78:VAL:HG13	2:D:602:ADP:N6	2.29	0.48
1:C:400:GLU:HB2	1:C:406:GLN:NE2	2.28	0.48
1:B:361:LYS:NZ	1:B:403:ILE:HA	2.29	0.48
1:A:125:LYS:HG2	1:A:314:LEU:HD22	1.95	0.47
1:B:370:ARG:CG	2:B:601:ADP:H5'1	2.45	0.47
1:D:73:HIS:HB3	1:D:135:LEU:HD22	1.97	0.47
1:F:172:ASP:OD2	1:F:175:LYS:HG3	2.14	0.47
1:D:346:VAL:HG21	1:D:387:LEU:HD11	1.94	0.47
1:B:142:MET:SD	1:C:303:GLU:HB2	2.54	0.47
1:B:169:CYS:O	1:B:170:ASP:HB2	2.14	0.47
1:B:346:VAL:HG21	1:B:387:LEU:HD11	1.97	0.47
1:E:343:LEU:HD13	1:F:101:ASN:HD22	1.78	0.47
1:A:150:GLU:CB	1:B:191:ARG:HH22	2.27	0.47
1:F:163:GLN:O	1:F:167:GLN:HG2	2.14	0.47
1:F:212:LEU:HD21	1:F:303:GLU:HG2	1.97	0.47
1:C:296:ILE:HG12	1:C:305:ILE:HD12	1.97	0.47
1:E:102:GLY:O	1:E:103:ASP:C	2.52	0.47
1:F:78:VAL:HG23	1:F:127:LEU:HD23	1.96	0.47
1:D:169:CYS:SG	1:D:175:LYS:CB	3.03	0.47
1:E:212:LEU:HD22	1:E:307:ARG:HE	1.80	0.47
1:E:214:LEU:O	1:E:240:THR:HB	2.15	0.47
1:B:347:ASP:O	1:B:394:GLU:HB2	2.15	0.47
1:C:149:THR:O	1:C:202:VAL:HB	2.15	0.47
1:C:261:ARG:HD3	1:C:294:ASP:OD1	2.15	0.47
1:C:190:SER:HB2	1:C:299:GLY:HA3	1.97	0.47
1:F:214:LEU:C	1:F:214:LEU:HD12	2.35	0.47
1:A:387:LEU:HB3	1:A:388:PRO:HD3	1.96	0.47
1:E:116:LEU:HD13	1:E:308:LEU:HD23	1.97	0.47
1:A:151:ALA:HB3	1:A:154:VAL:CB	2.33	0.47
1:C:70:ILE:O	1:C:74:LEU:HG	2.15	0.47
1:D:144:ASP:O	1:D:147:THR:CG2	2.54	0.47
1:D:332:ALA:O	1:D:336:GLN:HG3	2.15	0.46
1:E:319:GLU:OE2	1:E:360:LYS:HE2	2.16	0.46
1:B:301:ILE:HG12	1:B:304:PHE:HB2	1.95	0.46
1:C:138:VAL:HG11	1:C:178:ARG:O	2.15	0.46
1:D:165:LEU:O	1:D:165:LEU:HD23	2.15	0.46
1:E:104:THR:CG2	1:E:110:LEU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ILE:HA	1:F:164:LYS:HE2	1.97	0.46
1:C:383:THR:O	1:C:387:LEU:HB2	2.14	0.46
1:E:190:SER:OG	1:E:299:GLY:HA3	2.15	0.46
1:F:86:LYS:O	1:F:90:VAL:HG23	2.14	0.46
1:A:160:ASN:HA	1:A:163:GLN:HG2	1.96	0.46
1:A:217:GLY:HA3	1:A:241:SER:OG	2.16	0.46
1:B:230:HIS:N	1:B:231:PRO:CD	2.77	0.46
1:C:317:LEU:HD21	1:C:368:GLY:HA2	1.98	0.46
1:D:114:ASN:H	1:D:309:PRO:HD2	1.79	0.46
1:D:148:LEU:CD2	1:D:158:VAL:HG12	2.25	0.46
1:D:166:LEU:HD22	1:D:171:TYR:HA	1.96	0.46
1:D:90:VAL:HG12	1:D:94:ASN:ND2	2.29	0.46
1:A:151:ALA:CB	1:A:153:TYR:CZ	2.97	0.46
1:C:403:ILE:CG2	1:C:404:ASP:N	2.78	0.46
1:E:163:GLN:O	1:E:167:GLN:HG3	2.16	0.46
1:E:370:ARG:HA	1:E:370:ARG:HD3	1.76	0.46
1:F:170:ASP:O	1:F:171:TYR:HB2	2.14	0.46
1:A:182:TYR:HA	1:A:246:ILE:O	2.16	0.46
1:B:162:ILE:HD11	1:B:240:THR:HG22	1.98	0.46
1:C:169:CYS:O	1:C:170:ASP:HB3	2.16	0.46
1:D:340:LEU:HD21	1:E:94:ASN:ND2	2.31	0.46
1:A:79:ILE:H	2:A:600:ADP:HN62	1.64	0.46
1:C:174:GLN:HE21	1:C:178:ARG:HH11	1.62	0.46
1:C:158:VAL:HG12	1:C:214:LEU:HD13	1.98	0.46
1:E:149:THR:HB	1:E:189:ILE:HG22	1.96	0.46
1:F:117:LEU:HD23	1:F:312:ALA:HB3	1.96	0.46
1:F:205:GLU:O	1:F:208:GLN:HG2	2.16	0.46
1:F:114:ASN:HD22	1:F:307:ARG:HG3	1.80	0.46
1:A:108:VAL:HG12	1:A:109:GLU:H	1.81	0.46
1:B:371:GLY:O	1:B:375:ILE:HG13	2.16	0.46
1:B:170:ASP:OD2	1:C:219:VAL:HG13	2.15	0.46
1:D:161:ILE:HA	1:D:164:LYS:HD2	1.98	0.46
1:E:177:GLN:O	1:E:242:LYS:HG2	2.16	0.46
1:E:212:LEU:CD2	1:E:304:PHE:HA	2.45	0.46
1:A:151:ALA:CB	1:A:153:TYR:CE1	2.99	0.46
1:A:112:LYS:CE	1:A:307:ARG:HE	2.27	0.46
1:A:166:LEU:HD11	1:A:238:VAL:HG21	1.98	0.45
1:A:401:SER:O	1:A:405:GLY:HA2	2.15	0.45
1:C:92:VAL:CG1	1:C:136:LEU:HD11	2.46	0.45
1:F:124:GLY:O	1:F:128:LEU:HG	2.16	0.45
1:F:258:ILE:HG12	1:F:294:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:ASN:HB2	1:F:307:ARG:O	2.15	0.45
1:B:151:ALA:O	1:B:154:VAL:HG12	2.16	0.45
1:E:157:ASP:O	1:E:157:ASP:OD1	2.33	0.45
1:F:359:ALA:O	1:F:363:MET:HG3	2.15	0.45
1:A:261:ARG:NH2	1:A:291:GLU:HG3	2.31	0.45
1:C:257:VAL:HG13	1:C:297:LYS:HD3	1.99	0.45
1:D:73:HIS:HB3	1:D:135:LEU:CD2	2.47	0.45
1:B:338:GLN:O	1:B:342:ASN:HB2	2.17	0.45
1:C:149:THR:HA	1:C:207:VAL:HG21	1.98	0.45
1:F:73:HIS:HE1	1:F:131:THR:HG23	1.82	0.45
1:F:283:GLU:O	1:F:287:LEU:HD13	2.17	0.45
1:B:261:ARG:HD2	1:B:294:ASP:OD1	2.16	0.45
1:E:391:GLU:O	1:E:391:GLU:HG2	2.17	0.45
1:B:148:LEU:O	1:B:154:VAL:HB	2.16	0.45
1:B:205:GLU:HA	1:B:208:GLN:CG	2.42	0.45
1:C:114:ASN:HB2	1:C:307:ARG:O	2.16	0.45
1:C:78:VAL:HG22	1:C:127:LEU:HD23	1.98	0.45
1:E:371:GLY:O	1:E:375:ILE:HG13	2.17	0.45
1:E:212:LEU:HD21	1:E:304:PHE:CD1	2.46	0.45
1:E:114:ASN:ND2	1:E:215:ILE:HD13	2.31	0.45
1:F:156:GLU:HA	1:F:159:GLU:HG2	1.98	0.45
1:A:354:ALA:O	1:A:358:ILE:HG13	2.17	0.45
1:F:73:HIS:HB3	1:F:135:LEU:HD22	1.99	0.45
1:C:114:ASN:HB3	1:C:308:LEU:HD23	1.98	0.45
1:F:184:ASP:C	1:F:185:GLN:HG2	2.37	0.45
1:F:81:GLN:NE2	1:F:314:LEU:HB3	2.31	0.45
1:A:195:ASN:N	1:A:196:PRO:CD	2.80	0.45
1:B:354:ALA:O	1:B:358:ILE:HG13	2.17	0.45
1:D:66:THR:CG2	1:D:69:GLU:HB2	2.47	0.45
1:E:327:LYS:HD3	1:E:355:LEU:HD13	1.99	0.45
1:F:296:ILE:HD11	1:F:302:PRO:HA	1.97	0.45
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.82	0.44
1:B:347:ASP:HB3	1:B:394:GLU:HB2	1.98	0.44
1:C:145:ALA:HB1	1:C:189:ILE:CG2	2.47	0.44
1:C:317:LEU:HB2	1:C:363:MET:HG2	1.99	0.44
1:E:251:PHE:HB3	1:E:254:LEU:CB	2.47	0.44
1:E:75:ASP:HA	1:E:85:LYS:HZ3	1.82	0.44
1:B:173:VAL:HG13	1:B:238:VAL:HB	1.98	0.44
1:D:83:GLN:O	1:D:87:VAL:HG23	2.17	0.44
1:E:151:ALA:C	1:E:154:VAL:HG12	2.37	0.44
1:E:172:ASP:O	1:E:173:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ALA:CB	1:B:140:PHE:HB2	2.47	0.44
1:B:208:GLN:O	1:B:212:LEU:HB2	2.17	0.44
1:B:212:LEU:HD21	1:B:303:GLU:CG	2.48	0.44
1:E:104:THR:HG21	1:E:109:GLU:HB2	1.98	0.44
1:E:131:THR:O	1:E:135:LEU:HG	2.18	0.44
1:E:163:GLN:NE2	1:E:166:LEU:HD11	2.33	0.44
1:E:387:LEU:N	1:E:388:PRO:CD	2.80	0.44
1:F:254:LEU:HA	1:F:257:VAL:HG12	1.99	0.44
1:F:71:ARG:NH2	1:F:82:GLU:OE1	2.50	0.44
1:A:301:ILE:HG13	1:A:304:PHE:H	1.81	0.44
1:B:232:GLN:C	1:B:233:GLN:HG3	2.37	0.44
1:D:117:LEU:HD23	1:D:312:ALA:HB3	1.98	0.44
1:A:151:ALA:HB1	1:A:153:TYR:CG	2.53	0.44
1:A:148:LEU:CA	1:A:154:VAL:HG21	2.39	0.44
1:E:386:ASP:HB3	1:F:68:HIS:CE1	2.51	0.44
1:F:177:GLN:CG	1:F:238:VAL:HG13	2.47	0.44
1:D:190:SER:OG	1:D:299:GLY:HA3	2.17	0.44
1:D:75:ASP:HA	1:D:85:LYS:HZ3	1.81	0.44
1:E:114:ASN:HB2	1:E:307:ARG:O	2.17	0.44
1:A:307:ARG:C	1:A:309:PRO:HD3	2.38	0.43
1:D:79:ILE:HD12	1:D:325:ILE:HA	2.00	0.43
1:E:110:LEU:CB	1:E:112:LYS:HE2	2.48	0.43
1:C:317:LEU:CD2	1:C:368:GLY:HA2	2.49	0.43
1:C:356:ASP:O	1:C:360:LYS:HG3	2.17	0.43
1:D:202:VAL:C	1:D:204:GLY:N	2.71	0.43
1:D:212:LEU:HD23	1:D:212:LEU:C	2.38	0.43
1:B:365:ARG:HG3	1:B:367:THR:CG2	2.47	0.43
1:D:114:ASN:HB2	1:D:307:ARG:O	2.18	0.43
1:E:344:GLU:OE2	1:E:388:PRO:HG3	2.18	0.43
1:F:361:LYS:HD3	1:F:365:ARG:NH2	2.34	0.43
1:B:324:GLN:HG3	1:B:328:GLU:OE2	2.18	0.43
1:D:204:GLY:O	1:D:207:VAL:N	2.50	0.43
1:E:258:ILE:HD12	1:E:290:VAL:HA	2.00	0.43
1:A:254:LEU:O	1:A:258:ILE:HG13	2.19	0.43
1:B:296:ILE:HD12	1:B:302:PRO:HG3	2.01	0.43
1:C:64:LEU:HD22	1:C:100:ARG:HD2	2.00	0.43
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.83	0.43
1:C:136:LEU:HB3	1:C:138:VAL:HG23	2.00	0.43
1:D:222:VAL:CG1	1:D:223:PRO:HD3	2.49	0.43
1:D:357:ALA:HB1	1:D:403:ILE:CG1	2.42	0.43
1:D:393:VAL:CB	1:D:414:GLY:HA3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:VAL:O	1:E:85:LYS:NZ	2.51	0.43
1:F:220:ALA:HA	1:F:237:GLN:CD	2.39	0.43
1:B:232:GLN:HB3	1:B:235:PHE:HB3	2.00	0.43
1:B:388:PRO:HG2	1:C:67:PRO:CD	2.49	0.43
1:C:195:ASN:HA	1:C:196:PRO:HD2	1.83	0.43
1:C:392:ASP:N	1:C:392:ASP:OD1	2.48	0.43
1:F:201:ASP:OD1	1:F:202:VAL:HG23	2.19	0.43
1:A:149:THR:N	1:A:207:VAL:HG21	2.33	0.43
1:D:175:LYS:HA	1:D:178:ARG:HD2	2.00	0.43
1:D:88:LEU:HD23	1:D:115:ILE:HD13	2.01	0.43
1:E:155:GLY:O	1:E:158:VAL:HB	2.19	0.43
1:E:295:LEU:HB2	1:E:305:ILE:HD13	2.00	0.43
1:D:326:LEU:O	1:D:332:ALA:HB1	2.18	0.43
1:D:386:ASP:HA	1:E:68:HIS:CD2	2.53	0.43
1:E:343:LEU:HD22	1:F:101:ASN:ND2	2.33	0.43
1:F:146:THR:HG23	1:F:185:GLN:HB3	2.01	0.43
1:A:86:LYS:HG3	1:F:385:TYR:CD1	2.54	0.43
1:A:186:ILE:O	1:A:189:ILE:HG12	2.19	0.43
1:D:167:GLN:CG	1:D:168:LYS:N	2.81	0.43
1:C:367:THR:CB	1:D:291:GLU:HG2	2.47	0.43
1:E:157:ASP:C	1:E:160:ASN:H	2.22	0.43
1:D:173:VAL:O	1:D:177:GLN:HG2	2.19	0.42
1:D:208:GLN:O	1:D:212:LEU:N	2.52	0.42
1:D:221:ALA:CB	1:D:223:PRO:HD2	2.49	0.42
1:F:156:GLU:O	1:F:159:GLU:HG2	2.19	0.42
1:F:142:MET:HG3	1:F:182:TYR:HD2	1.84	0.42
1:F:95:HIS:NE2	1:F:244:LEU:HB2	2.34	0.42
1:B:118:ILE:O	1:B:313:THR:HA	2.19	0.42
1:C:116:LEU:HD12	1:C:247:CYS:O	2.19	0.42
1:D:160:ASN:O	1:D:163:GLN:HB3	2.19	0.42
1:D:125:LYS:HG2	1:D:314:LEU:CD1	2.49	0.42
1:E:160:ASN:HA	1:E:163:GLN:HB3	2.01	0.42
1:F:184:ASP:OD1	1:F:185:GLN:N	2.52	0.42
1:F:406:GLN:HG3	1:F:407:SER:N	2.35	0.42
1:A:92:VAL:HG21	1:A:132:LEU:HD22	2.02	0.42
1:B:75:ASP:OD1	1:B:85:LYS:HE2	2.18	0.42
1:C:347:ASP:O	1:C:394:GLU:HB2	2.19	0.42
1:A:131:THR:O	1:A:135:LEU:HG	2.20	0.42
1:A:398:ILE:HG13	1:A:400:GLU:N	2.34	0.42
1:D:133:ALA:CB	1:D:140:PHE:HB2	2.49	0.42
1:E:154:VAL:O	1:E:154:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:VAL:O	1:E:158:VAL:N	2.52	0.42
1:F:186:ILE:HD13	1:F:247:CYS:HB3	2.02	0.42
1:A:163:GLN:HG3	1:A:164:LYS:N	2.35	0.42
1:B:235:PHE:O	1:B:238:VAL:HG12	2.18	0.42
1:E:103:ASP:C	1:E:104:THR:HG23	2.40	0.42
1:B:99:LEU:HD22	1:B:242:LYS:HD2	2.01	0.42
1:B:361:LYS:HB2	1:B:361:LYS:HE3	1.89	0.42
1:D:221:ALA:HB3	1:D:223:PRO:HD2	2.02	0.42
1:A:86:LYS:HD2	1:F:381:LEU:CD1	2.50	0.42
1:D:189:ILE:CD1	1:D:208:GLN:HG3	2.49	0.42
1:D:79:ILE:HD11	1:D:329:PRO:HD3	2.02	0.42
1:E:326:LEU:O	1:E:332:ALA:HB1	2.20	0.42
1:A:141:THR:HB	1:A:168:LYS:HE3	2.02	0.42
1:C:360:LYS:HA	1:C:363:MET:CE	2.50	0.42
1:D:179:GLY:O	1:D:243:ILE:HG23	2.20	0.42
1:E:151:ALA:O	1:E:154:VAL:CG1	2.58	0.42
1:B:403:ILE:HG23	1:B:404:ASP:N	2.34	0.42
1:C:135:LEU:C	1:C:135:LEU:HD12	2.39	0.42
1:F:341:PHE:CD1	1:F:348:LEU:HD22	2.54	0.42
1:A:369:ALA:HA	1:A:372:LEU:HG	2.02	0.41
1:C:371:GLY:O	1:C:375:ILE:HG13	2.20	0.41
1:E:104:THR:OG1	1:E:107:GLY:N	2.53	0.41
1:E:114:ASN:HD21	1:E:215:ILE:HD13	1.84	0.41
1:F:154:VAL:HG12	1:F:154:VAL:O	2.20	0.41
1:A:162:ILE:O	1:A:166:LEU:HD13	2.20	0.41
1:C:135:LEU:HD12	1:C:136:LEU:N	2.34	0.41
1:D:66:THR:HG22	1:D:69:GLU:HB2	2.01	0.41
1:B:166:LEU:HD22	1:B:171:TYR:HA	2.01	0.41
1:D:189:ILE:HG12	1:D:208:GLN:HE21	1.86	0.41
1:B:295:LEU:HB2	1:B:305:ILE:HD13	2.02	0.41
1:D:380:LEU:O	1:D:384:MET:HG3	2.20	0.41
1:F:105:SER:O	1:F:106:ASN:HB2	2.21	0.41
1:F:347:ASP:O	1:F:394:GLU:HB2	2.20	0.41
1:A:177:GLN:HA	1:A:243:ILE:HG22	2.02	0.41
1:A:391:GLU:HG2	1:A:391:GLU:O	2.20	0.41
1:C:199:THR:HG22	1:C:201:ASP:N	2.35	0.41
1:E:254:LEU:HA	1:E:257:VAL:HG12	2.02	0.41
1:A:208:GLN:O	1:A:212:LEU:HB2	2.20	0.41
1:C:346:VAL:HG21	1:C:387:LEU:HD11	2.03	0.41
1:D:173:VAL:HG13	1:D:237:GLN:O	2.21	0.41
1:A:371:GLY:O	1:A:375:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LEU:HD22	1:D:304:PHE:HD2	1.85	0.41
1:E:159:GLU:HB2	1:E:235:PHE:CE1	2.56	0.41
1:E:76:ASP:O	1:E:329:PRO:HA	2.21	0.41
1:A:386:ASP:HB3	1:B:68:HIS:NE2	2.35	0.41
1:E:144:ASP:HB3	1:E:147:THR:HG23	2.02	0.41
1:E:173:VAL:HG21	1:E:237:GLN:HB3	2.03	0.41
1:E:382:ASP:O	1:E:385:TYR:HB3	2.21	0.41
1:F:146:THR:HG23	1:F:185:GLN:CB	2.51	0.41
1:A:151:ALA:HB2	1:A:153:TYR:CE1	2.56	0.41
1:A:251:PHE:HB3	1:A:254:LEU:CB	2.51	0.41
1:B:216:GLU:CD	1:B:307:ARG:HD2	2.41	0.41
1:B:212:LEU:HD21	1:B:303:GLU:HG3	2.03	0.41
1:B:369:ALA:HB3	2:B:601:ADP:C8	2.55	0.41
1:E:346:VAL:HG21	1:E:387:LEU:HD11	2.03	0.41
1:E:363:MET:HB2	1:E:363:MET:HE2	1.86	0.41
1:F:114:ASN:HB3	1:F:308:LEU:CD1	2.48	0.41
1:A:396:VAL:HB	1:A:410:LEU:HB3	2.03	0.41
1:B:207:VAL:HG12	1:B:211:LEU:HD22	2.03	0.41
1:B:301:ILE:HG13	1:B:304:PHE:H	1.84	0.41
1:B:370:ARG:HG3	2:B:601:ADP:H5'1	2.02	0.41
1:C:380:LEU:O	1:C:384:MET:HG3	2.21	0.41
1:D:202:VAL:O	1:D:202:VAL:HG12	2.21	0.41
1:A:296:ILE:HD11	1:A:302:PRO:HA	2.03	0.41
1:C:250:ALA:O	5:C:803:HOH:O	2.22	0.41
1:C:391:GLU:O	1:C:391:GLU:HG2	2.21	0.41
1:E:146:THR:O	1:E:149:THR:HG22	2.21	0.41
1:E:173:VAL:CG1	1:E:238:VAL:HB	2.38	0.41
1:B:151:ALA:HB1	1:B:153:TYR:CE1	2.57	0.40
1:C:333:LEU:HD22	1:C:337:TYR:HE1	1.86	0.40
1:E:104:THR:OG1	1:E:107:GLY:CA	2.69	0.40
1:E:141:THR:CG2	1:E:181:VAL:HG22	2.51	0.40
1:F:153:TYR:O	1:F:154:VAL:CB	2.68	0.40
1:C:367:THR:CG2	1:D:291:GLU:HG2	2.51	0.40
1:D:101:ASN:OD1	1:D:101:ASN:C	2.59	0.40
1:D:116:LEU:HD12	1:D:247:CYS:O	2.21	0.40
1:D:254:LEU:HG	1:D:258:ILE:HD11	2.02	0.40
1:E:329:PRO:CG	2:E:603:ADP:H2	2.34	0.40
1:F:104:THR:O	1:F:105:SER:HB2	2.21	0.40
1:A:261:ARG:HH21	1:F:365:ARG:HB3	1.86	0.40
1:B:251:PHE:HB3	1:B:254:LEU:HB2	2.03	0.40
1:B:321:ALA:O	1:B:325:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:NE2	1:C:316:GLU:H	2.15	0.40
1:C:404:ASP:C	1:C:406:GLN:N	2.74	0.40
1:D:206:GLY:O	1:D:209:GLN:HB3	2.20	0.40
1:E:117:LEU:HD23	1:E:312:ALA:HB3	2.02	0.40
1:F:326:LEU:O	1:F:332:ALA:HB1	2.22	0.40
1:F:84:ALA:O	1:F:88:LEU:HD13	2.22	0.40
1:A:149:THR:O	1:A:150:GLU:CB	2.70	0.40
1:C:187:ASP:HB3	1:C:251:PHE:CD2	2.56	0.40
1:C:307:ARG:C	1:C:309:PRO:HD3	2.41	0.40
1:E:322:LEU:HA	1:E:325:ILE:HD12	2.04	0.40
1:B:388:PRO:HG2	1:C:67:PRO:HD2	2.04	0.40
1:C:301:ILE:HG13	1:C:304:PHE:H	1.86	0.40
1:C:317:LEU:HD11	1:C:368:GLY:HA2	2.02	0.40
1:D:347:ASP:O	1:D:394:GLU:HB2	2.20	0.40
1:E:158:VAL:HG12	1:E:214:LEU:HD13	2.03	0.40
1:E:257:VAL:HG21	1:E:297:LYS:HB2	2.02	0.40
1:F:187:ASP:OD1	1:F:187:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/363 (86%)	298 (96%)	14 (4%)	0	100	100
1	B	307/363 (85%)	298 (97%)	8 (3%)	1 (0%)	44	79
1	C	297/363 (82%)	290 (98%)	6 (2%)	1 (0%)	44	79
1	D	308/363 (85%)	301 (98%)	6 (2%)	1 (0%)	44	79
1	E	305/363 (84%)	297 (97%)	8 (3%)	0	100	100
1	F	302/363 (83%)	292 (97%)	9 (3%)	1 (0%)	44	79
All	All	1831/2178 (84%)	1776 (97%)	51 (3%)	4 (0%)	51	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	154	VAL
1	D	154	VAL
1	C	103	ASP
1	B	231	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/299 (82%)	238 (98%)	6 (2%)	53	81
1	B	250/299 (84%)	248 (99%)	2 (1%)	85	93
1	C	248/299 (83%)	245 (99%)	3 (1%)	75	89
1	D	235/299 (79%)	235 (100%)	0	100	100
1	E	235/299 (79%)	233 (99%)	2 (1%)	82	92
1	F	246/299 (82%)	243 (99%)	3 (1%)	75	89
All	All	1458/1794 (81%)	1442 (99%)	16 (1%)	78	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	A	157	ASP
1	A	170	ASP
1	A	243	ILE
1	A	391	GLU
1	A	403	ILE
1	B	170	ASP
1	B	211	LEU
1	C	315	ASN
1	C	386	ASP
1	C	398	ILE
1	E	109	GLU
1	E	157	ASP

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Mol	Chain	Res	Type
1	F	68	HIS
1	F	103	ASP
1	F	148	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	101	ASN
1	A	114	ASN
1	B	209	GLN
1	C	101	ASN
1	C	174	GLN
1	C	315	ASN
1	C	406	GLN
1	D	73	HIS
1	D	94	ASN
1	D	114	ASN
1	D	209	GLN
1	E	114	ASN
1	E	209	GLN
1	E	260	HIS
1	F	73	HIS
1	F	81	GLN
1	F	101	ASN
1	F	114	ASN
1	F	160	ASN
1	F	260	HIS
1	F	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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	ADP	A	600	-	25,29,29	1.16	2 (8%)	24,45,45	1.70	4 (16%)
3	SO4	A	700	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	A	701	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	A	705	-	4,4,4	0.16	0	6,6,6	0.06	0
2	ADP	B	601	-	25,29,29	1.16	2 (8%)	24,45,45	1.69	4 (16%)
3	SO4	B	702	-	4,4,4	0.17	0	6,6,6	0.05	0
3	SO4	B	707	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	B	708	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	B	709	-	4,4,4	0.13	0	6,6,6	0.15	0
3	SO4	C	500	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	C	703	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	C	704	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	C	706	-	4,4,4	0.15	0	6,6,6	0.08	0
2	ADP	D	602	-	25,29,29	1.16	2 (8%)	24,45,45	1.71	4 (16%)
3	SO4	D	710	-	4,4,4	1.01	0	6,6,6	1.58	1 (16%)
2	ADP	E	603	-	25,29,29	1.16	2 (8%)	24,45,45	1.66	4 (16%)
3	SO4	F	500	-	4,4,4	0.14	0	6,6,6	0.12	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	ADP	A	600	-	-	0/12/32/32	0/3/3/3
3	SO4	A	700	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	A	705	-	-	0/0/0/0	0/0/0/0
2	ADP	B	601	-	-	0/12/32/32	0/3/3/3
3	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	SO4	B	707	-	-	0/0/0/0	0/0/0/0
3	SO4	B	708	-	-	0/0/0/0	0/0/0/0
3	SO4	B	709	-	-	0/0/0/0	0/0/0/0
3	SO4	C	500	-	-	0/0/0/0	0/0/0/0
3	SO4	C	703	-	-	0/0/0/0	0/0/0/0
3	SO4	C	704	-	-	0/0/0/0	0/0/0/0
3	SO4	C	706	-	-	0/0/0/0	0/0/0/0
2	ADP	D	602	-	-	0/12/32/32	0/3/3/3
3	SO4	D	710	-	-	0/0/0/0	0/0/0/0
2	ADP	E	603	-	-	0/12/32/32	0/3/3/3
3	SO4	F	500	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	603	ADP	C2-N3	2.01	1.35	1.32
2	D	602	ADP	C2-N3	2.01	1.35	1.32
2	B	601	ADP	C2-N3	2.06	1.35	1.32
2	A	600	ADP	O4'-C1'	2.11	1.44	1.41
2	A	600	ADP	C5-C4	3.26	1.47	1.40
2	B	601	ADP	C5-C4	3.34	1.48	1.40
2	E	603	ADP	C5-C4	3.37	1.48	1.40
2	D	602	ADP	C5-C4	3.40	1.48	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	ADP	N3-C2-N1	-5.89	123.72	128.86
2	A	600	ADP	N3-C2-N1	-5.73	123.87	128.86
2	B	601	ADP	N3-C2-N1	-5.65	123.94	128.86
2	E	603	ADP	N3-C2-N1	-5.49	124.07	128.86
2	B	601	ADP	C4-C5-N7	-3.32	106.20	109.41
2	E	603	ADP	C4-C5-N7	-3.25	106.27	109.41
2	A	600	ADP	C4-C5-N7	-3.15	106.37	109.41
2	D	602	ADP	C4-C5-N7	-3.14	106.37	109.41
2	E	603	ADP	C2'-C3'-C4'	2.10	106.70	102.62
2	E	603	ADP	C4'-O4'-C1'	2.10	112.00	109.77
2	D	602	ADP	C2'-C3'-C4'	2.13	106.76	102.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C2'-C3'-C4'	2.20	106.91	102.62
2	B	601	ADP	C4'-O4'-C1'	2.21	112.12	109.77
2	A	600	ADP	C4'-O4'-C1'	2.22	112.14	109.77
2	D	602	ADP	C4'-O4'-C1'	2.24	112.15	109.77
2	A	600	ADP	C2'-C3'-C4'	2.40	107.29	102.62
3	D	710	SO4	O4-S-O3	3.65	125.40	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	ADP	1	0
2	B	601	ADP	3	0
2	D	602	ADP	4	0
2	E	603	ADP	9	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/363 (88%)	0.41	30 (9%) 9 7	62, 109, 241, 416	0
1	B	315/363 (86%)	0.35	25 (7%) 13 10	63, 120, 211, 373	0
1	C	307/363 (84%)	0.32	20 (6%) 20 15	67, 123, 226, 412	0
1	D	316/363 (87%)	0.59	36 (11%) 6 4	72, 139, 235, 357	0
1	E	313/363 (86%)	0.56	34 (10%) 6 5	74, 146, 301, 440	0
1	F	314/363 (86%)	0.55	34 (10%) 6 5	65, 140, 272, 354	0
All	All	1885/2178 (86%)	0.47	179 (9%) 9 7	62, 130, 249, 440	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	SER	15.9
1	F	223	PRO	11.8
1	D	150	GLU	10.8
1	E	106	ASN	9.4
1	F	281	ALA	9.0
1	F	220	ALA	8.9
1	E	266	SER	8.1
1	F	106	ASN	7.7
1	D	149	THR	7.6
1	D	237	GLN	7.4
1	A	149	THR	7.3
1	E	156	GLU	7.2
1	D	238	VAL	7.1
1	C	154	VAL	6.9
1	D	151	ALA	6.8
1	D	62	SER	6.6
1	F	104	THR	6.6
1	F	105	SER	6.6
1	E	155	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	176	ALA	5.7
1	B	151	ALA	5.6
1	A	194	ASP	5.4
1	E	103	ASP	5.4
1	B	171	TYR	5.4
1	C	197	SER	5.3
1	C	199	THR	5.3
1	A	150	GLU	5.3
1	D	265	GLY	5.3
1	F	107	GLY	5.3
1	E	237	GLN	5.2
1	D	104	THR	5.2
1	A	153	TYR	5.2
1	B	101	ASN	5.1
1	A	103	ASP	5.1
1	D	103	ASP	5.1
1	B	392	ASP	4.9
1	A	196	PRO	4.9
1	B	390	MET	4.8
1	E	173	VAL	4.7
1	D	264	THR	4.6
1	C	195	ASN	4.6
1	F	222	VAL	4.5
1	E	220	ALA	4.5
1	C	289	GLN	4.4
1	E	105	SER	4.3
1	D	403	ILE	4.3
1	C	103	ASP	4.2
1	C	153	TYR	4.2
1	E	217	GLY	4.2
1	E	392	ASP	4.1
1	D	155	GLY	4.0
1	A	238	VAL	3.9
1	C	111	GLY	3.9
1	B	228	ARG	3.8
1	F	282	SER	3.8
1	D	186	ILE	3.8
1	D	156	GLU	3.8
1	A	151	ALA	3.7
1	A	155	GLY	3.7
1	F	234	GLU	3.7
1	E	104	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	173	VAL	3.6
1	F	260	HIS	3.6
1	D	222	VAL	3.5
1	A	171	TYR	3.5
1	A	204	GLY	3.5
1	E	262	VAL	3.5
1	A	169	CYS	3.5
1	C	198	ILE	3.5
1	D	390	MET	3.4
1	B	414	GLY	3.4
1	F	219	VAL	3.4
1	E	221	ALA	3.3
1	F	152	GLY	3.3
1	B	254	LEU	3.3
1	D	223	PRO	3.2
1	F	101	ASN	3.2
1	D	211	LEU	3.2
1	A	203	SER	3.2
1	E	258	ILE	3.1
1	A	195	ASN	3.1
1	C	155	GLY	3.1
1	E	219	VAL	3.1
1	F	200	ARG	3.1
1	D	415	LYS	3.1
1	E	188	LYS	3.1
1	F	153	TYR	3.0
1	F	102	GLY	3.0
1	D	162	ILE	3.0
1	B	173	VAL	3.0
1	D	220	ALA	3.0
1	A	280	LYS	3.0
1	D	254	LEU	3.0
1	C	149	THR	2.9
1	E	330	LYS	2.9
1	C	104	THR	2.9
1	D	239	ASP	2.9
1	B	150	GLU	2.9
1	D	101	ASN	2.8
1	D	221	ALA	2.8
1	D	331	ASN	2.7
1	E	109	GLU	2.7
1	A	106	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	218	THR	2.7
1	F	149	THR	2.7
1	F	108	VAL	2.7
1	E	153	TYR	2.7
1	B	286	LEU	2.7
1	F	218	THR	2.6
1	B	106	ASN	2.6
1	E	149	THR	2.6
1	B	109	GLU	2.6
1	F	347	ASP	2.6
1	F	112	LYS	2.6
1	C	172	ASP	2.5
1	D	105	SER	2.5
1	D	171	TYR	2.5
1	C	156	GLU	2.5
1	A	107	GLY	2.5
1	B	264	THR	2.5
1	D	147	THR	2.5
1	F	235	PHE	2.5
1	D	152	GLY	2.5
1	A	156	GLU	2.5
1	E	205	GLU	2.5
1	F	204	GLY	2.4
1	A	174	GLN	2.4
1	E	175	LYS	2.4
1	D	391	GLU	2.4
1	F	258	ILE	2.4
1	A	200	ARG	2.4
1	A	237	GLN	2.4
1	A	265	GLY	2.4
1	B	413	TYR	2.4
1	F	203	SER	2.3
1	A	266	SER	2.3
1	D	207	VAL	2.3
1	C	174	GLN	2.3
1	D	189	ILE	2.3
1	D	253	GLY	2.3
1	E	365	ARG	2.3
1	C	404	ASP	2.3
1	D	304	PHE	2.3
1	B	205	GLU	2.2
1	F	284	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	298	PHE	2.2
1	F	257	VAL	2.2
1	E	145	ALA	2.2
1	B	153	TYR	2.2
1	A	105	SER	2.2
1	D	153	TYR	2.2
1	E	414	GLY	2.2
1	C	344	GLU	2.2
1	B	411	LEU	2.2
1	B	403	ILE	2.1
1	E	265	GLY	2.1
1	B	253	GLY	2.1
1	B	410	LEU	2.1
1	E	179	GLY	2.1
1	E	206	GLY	2.1
1	E	113	SER	2.1
1	C	392	ASP	2.1
1	A	257	VAL	2.1
1	F	295	LEU	2.1
1	B	159	GLU	2.1
1	A	172	ASP	2.1
1	B	396	VAL	2.1
1	C	201	ASP	2.1
1	B	399	ASP	2.1
1	C	294	ASP	2.1
1	F	63	ALA	2.1
1	B	105	SER	2.1
1	F	405	GLY	2.1
1	F	81	GLN	2.0
1	E	64	LEU	2.0
1	A	392	ASP	2.0
1	F	297	LYS	2.0
1	E	159	GLU	2.0
1	A	192	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	D	710	5/5	0.69	0.43	5.88	190,190,190,190	0
3	SO4	B	702	5/5	0.58	0.35	3.78	191,191,191,191	0
2	ADP	D	602	27/27	0.88	0.34	2.14	132,153,162,170	16
2	ADP	E	603	27/27	0.89	0.29	1.06	135,151,159,166	14
2	ADP	B	601	27/27	0.93	0.26	0.98	95,119,137,139	10
2	ADP	A	600	27/27	0.90	0.25	0.85	78,93,113,120	9
3	SO4	F	500	5/5	0.95	0.23	0.77	96,96,96,96	0
3	SO4	C	500	5/5	0.95	0.25	0.36	100,100,100,100	0
4	MG	D	900	1/1	0.86	0.21	-0.44	107,107,107,107	0
3	SO4	C	703	5/5	0.90	0.19	-0.71	169,169,169,169	0
4	MG	B	901	1/1	0.88	0.90	-	115,115,115,115	0
3	SO4	C	706	5/5	0.77	0.22	-	232,232,232,232	0
3	SO4	B	708	5/5	0.78	0.97	-	231,231,231,231	0
3	SO4	C	704	5/5	0.63	0.38	-	233,233,233,233	0
3	SO4	A	705	5/5	0.83	0.19	-	173,173,173,173	0
3	SO4	B	707	5/5	0.82	0.27	-	179,179,179,179	0
3	SO4	A	700	5/5	0.92	0.22	-	147,147,147,147	0
3	SO4	B	709	5/5	0.85	0.54	-	178,178,178,178	0
3	SO4	A	701	5/5	0.82	0.21	-	168,168,168,168	0

6.5 Other polymers [i](#)

There are no such residues in this entry.