Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:06 PM GMT

PDB ID	:	4KI8
Title	:	Crystal structure of a GroEL-ADP complex in the relaxed allosteric state
Authors	:	Fei, X.; Yang, D.; LaRonde-LeBlanc, N.; Lorimer, G.H.
Deposited on	:	2013-05-01
Resolution	:	2.72 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

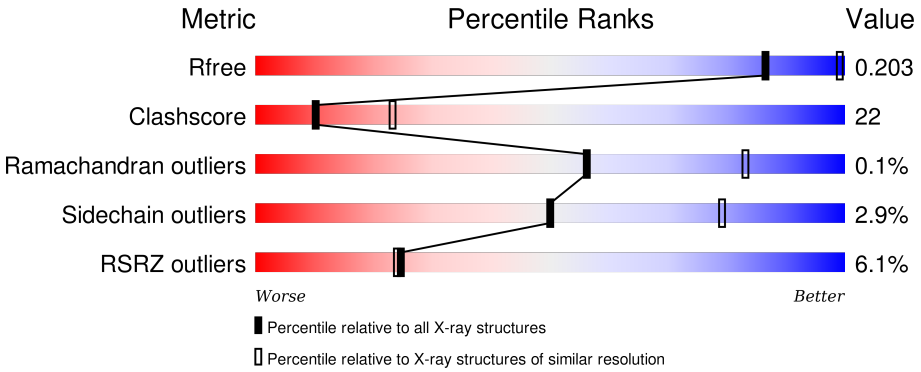
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.72 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	548	3% 68% 26%
1	B	548	4% 67% 27%
1	C	548	12% 62% 32%
1	D	548	2% 68% 26%
1	E	548	2% 68% 25%

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Mol	Chain	Length	Quality of chain
1	F	548	6% 64% 30%
1	G	548	11% 61% 33%

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	B	601	-	-	-	X
4	K	A	603	-	-	-	X
4	K	B	603	-	-	-	X
4	K	C	603	-	-	-	X
4	K	F	603	-	-	-	X
4	K	G	603	-	-	-	X
5	MPD	A	605	-	-	-	X
5	MPD	A	606	-	-	-	X
5	MPD	A	608	-	-	-	X
5	MPD	A	609	-	-	-	X
5	MPD	B	604	-	-	-	X
5	MPD	B	605	-	-	-	X
5	MPD	B	607	-	-	-	X
5	MPD	B	608	-	-	-	X
5	MPD	C	604	-	-	-	X
5	MPD	D	604	-	-	-	X
5	MPD	D	605	-	-	-	X
5	MPD	E	604	-	-	-	X
5	MPD	F	604	-	-	-	X
5	MPD	G	604	-	-	-	X
6	CA	D	607	-	-	-	X
6	CA	G	607	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27977 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.

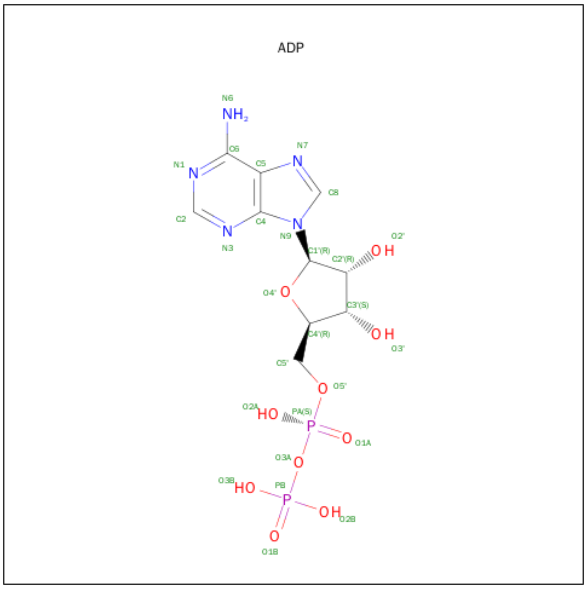
- Molecule 1 is a protein called GroEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			
1	B	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			
1	C	524	Total	C	N	O	S	0	3	0
			3864	2405	668	771	20			
1	D	524	Total	C	N	O	S	0	2	0
			3862	2403	668	771	20			
1	E	524	Total	C	N	O	S	0	1	0
			3851	2396	663	772	20			
1	F	524	Total	C	N	O	S	0	4	0
			3873	2410	668	775	20			
1	G	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
A	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
B	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
B	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
C	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
C	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
D	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
D	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
E	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
E	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
F	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
F	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
G	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
G	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1

- 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	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

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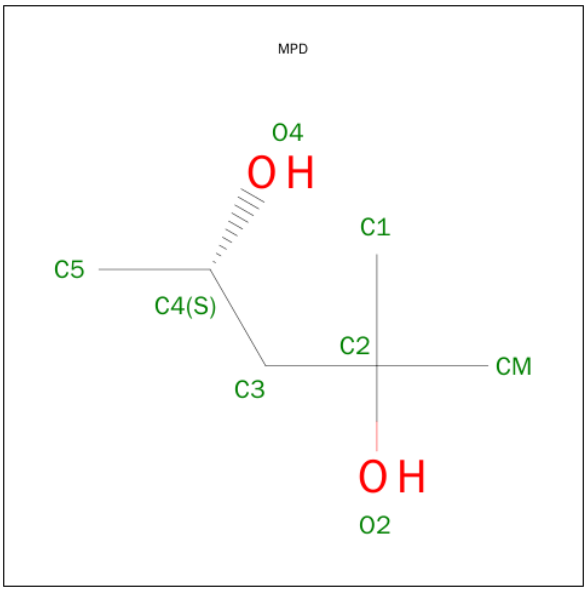
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total K 2 2	0	0
4	D	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0
4	F	2	Total K 2 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	F	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	3	Total Ca 3 3	0	0
6	D	1	Total Ca 1 1	0	0
6	E	3	Total Ca 3 3	0	0
6	B	1	Total Ca 1 1	0	0
6	A	2	Total Ca 2 2	0	0
6	F	1	Total Ca 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	90	Total O 90 90	0	0
7	B	112	Total O 112 112	0	0
7	C	88	Total O 88 88	0	0
7	D	90	Total O 90 90	0	0
7	E	65	Total O 65 65	0	0
7	F	67	Total O 67 67	0	0

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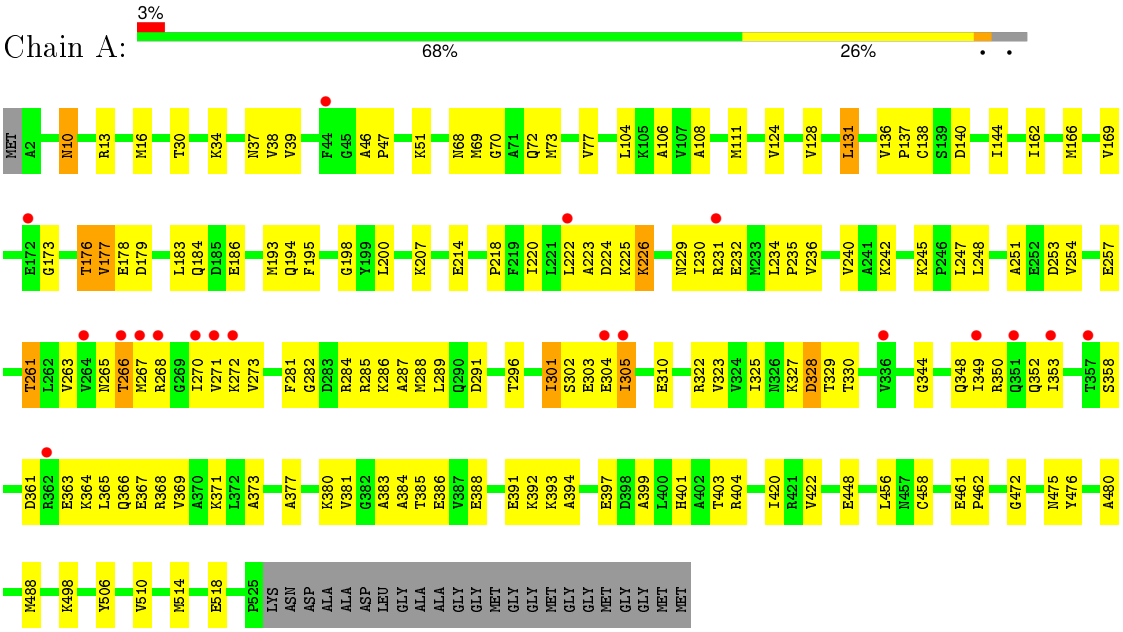
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	85	Total O 85 85	0	0

3 Residue-property plots (i)

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

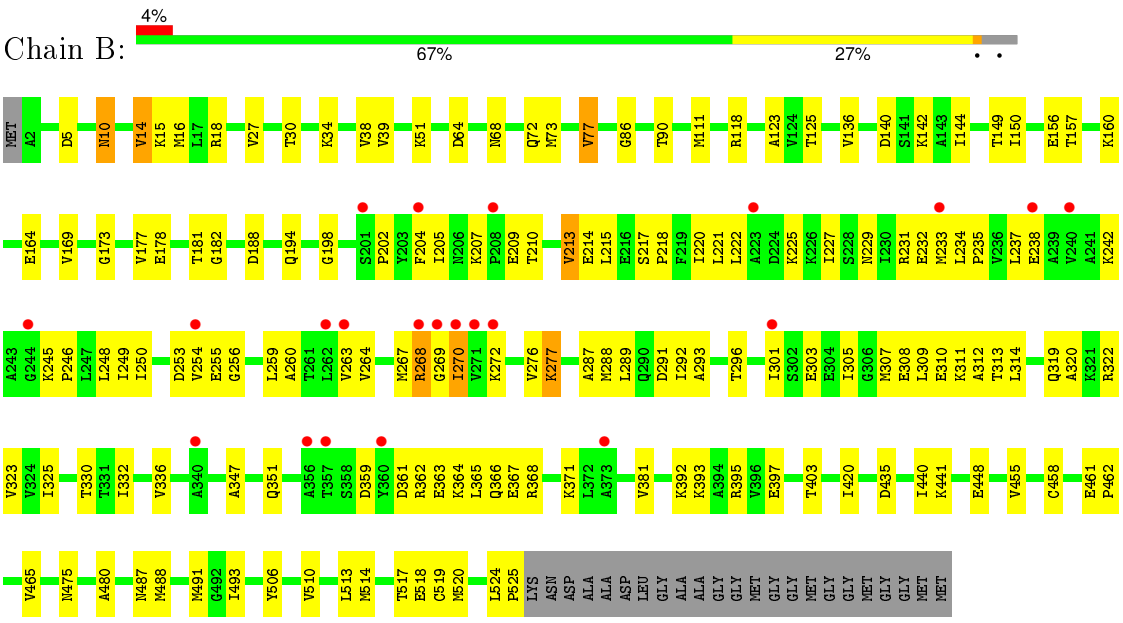
- Molecule 1: GroEL protein

Chain A:



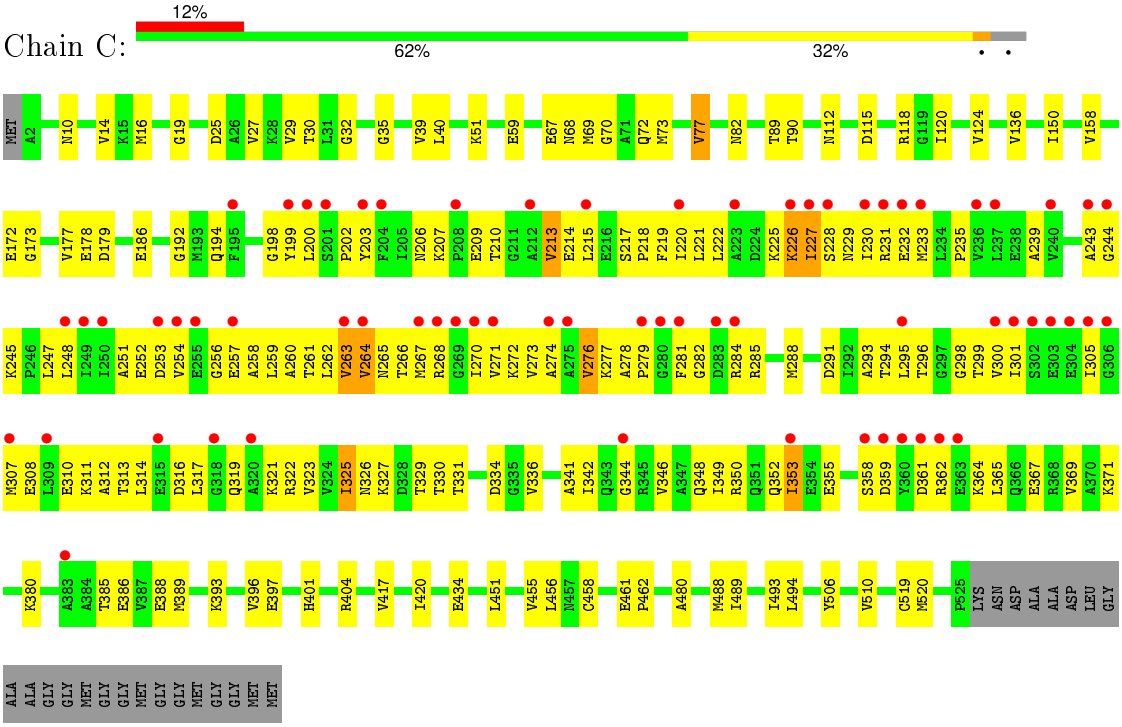
- Molecule 1: GroEL protein

Chain B:



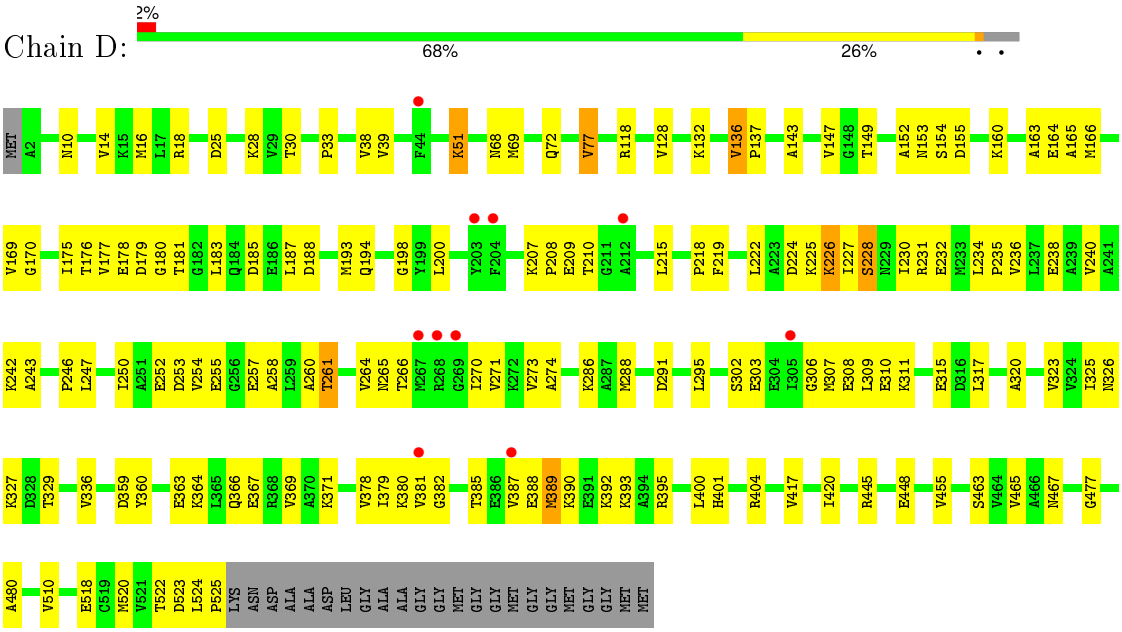
• Molecule 1: GroEL protein

Chain C:



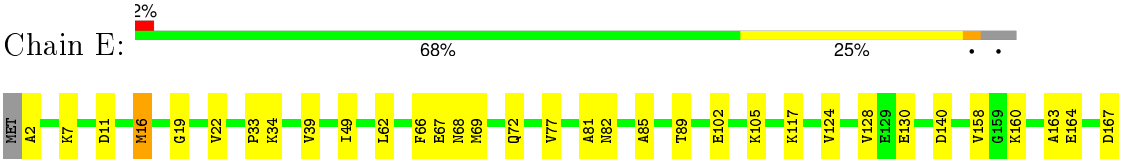
• Molecule 1: GroEL protein

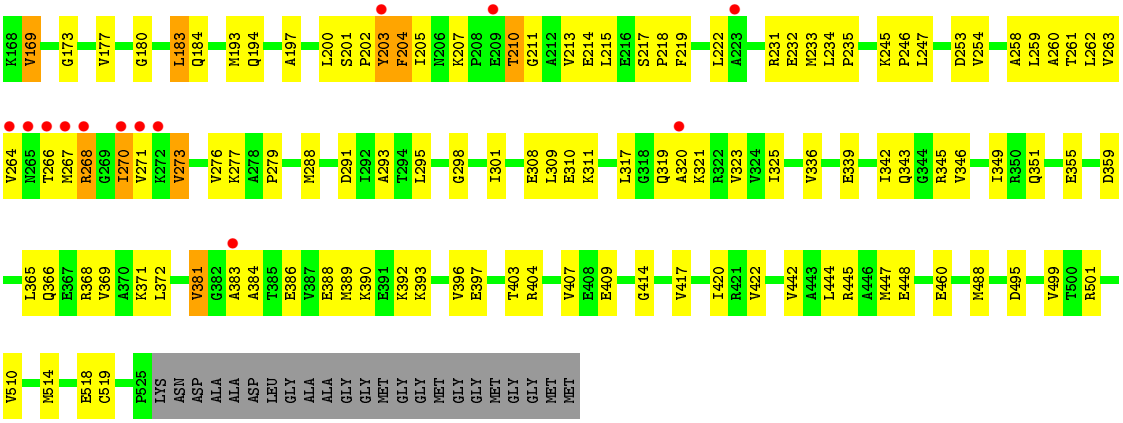
Chain D:



• Molecule 1: GroEL protein

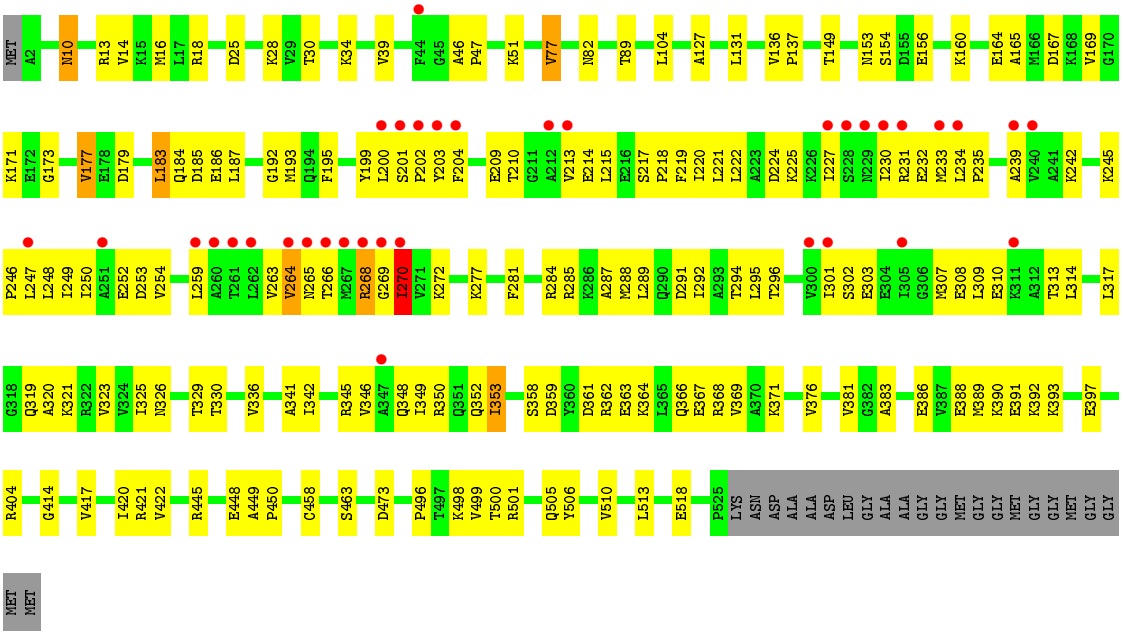
Chain E:





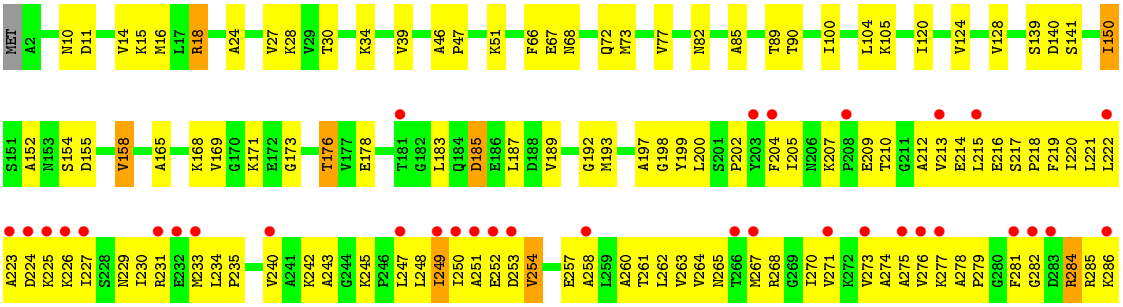
• Molecule 1: GroEL protein

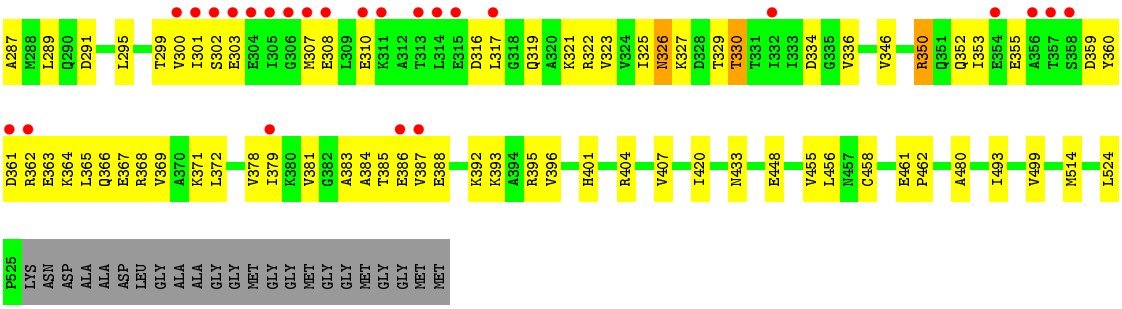
Chain F:



• Molecule 1: GroEL protein

Chain G:




A287 M288 L289 Q290 D291 L295 T299 V300 I301 S302 E303 E304 T305 G306 M307 E308 L309 E310 K311 A312 T313 L314 E315 D316 L317 G318 Q319 A320 K321 R322 V323 V324 I325 N326 K327 D328 T329 T330 T331 I332 I333 D334 G335 V336 V346 R350 Q351 Q352 I353 E354 E355 A356 T357 S358 D359 Y360
D361 R362 E363 K364 L365 Q366 E367 R368 V369 A370 K371 L372 V378 I379 K380 V381 G382 A383 A384 T385 E386 V387 E388 K392 K393 A394 R395 V396 H401 R404 V407 I420 N433 E448 V455 L456 N457 C458 E461 P462 A480 I493 V499 M514 L524
P525 LYS ASN ASP ALA ALA ASP LEU GLY ALA ALA GLY GLY MET GLY GLY MET GLY GLY MET GLY GLY MET MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.22Å 141.66Å 156.69Å 90.00° 113.84° 90.00°	Depositor
Resolution (Å)	46.17 – 2.72 46.17 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.17-2.72) 95.6 (46.17-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.166 , 0.203 0.165 , 0.203	Depositor DCC
R_{free} test set	1995 reflections (1.66%)	DCC
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 120262 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27977	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, MPD, CA, 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	0.28	0/3885	0.48	0/5246
1	B	0.29	0/3885	0.47	0/5246
1	C	0.32	0/3907	0.50	0/5274
1	D	0.28	0/3896	0.47	0/5260
1	E	0.27	0/3882	0.47	0/5243
1	F	0.28	0/3913	0.47	0/5284
1	G	0.27	0/3885	0.49	0/5246
All	All	0.29	0/27253	0.48	0/36799

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

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	3854	0	3982	154	0
1	B	3854	0	3982	147	0
1	C	3864	0	3994	249	1
1	D	3862	0	3995	126	0
1	E	3851	0	3975	121	0
1	F	3873	0	4005	180	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3854	0	3982	259	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	2	0
2	F	27	0	12	0	0
2	G	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
5	A	48	0	84	13	0
5	B	40	0	70	5	0
5	C	8	0	14	1	0
5	D	24	0	42	2	0
5	E	8	0	14	2	0
5	F	8	0	14	0	0
5	G	16	0	28	3	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
7	A	90	0	0	4	0
7	B	112	0	0	7	0
7	C	88	0	0	6	0
7	D	90	0	0	4	0
7	E	65	0	0	8	0
7	F	67	0	0	2	0
7	G	85	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27977	0	28265	1210	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1210) 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:A:230:ILE:HD12	1:A:261:THR:HG21	1.23	1.15
1:G:281:PHE:HB3	1:G:285:ARG:HB3	1.18	1.14
1:A:183:LEU:HA	1:A:383:ALA:HB2	1.14	1.09
1:B:255:GLU:HA	1:B:259:LEU:HD23	1.28	1.07
1:C:225:LYS:HB2	1:C:251:ALA:HB1	1.31	1.07
1:E:183:LEU:HD13	1:E:384:ALA:HB2	1.38	1.05
1:C:232:GLU:HB3	1:C:233:MET:HE2	1.37	1.04
1:A:383:ALA:HB1	1:A:384:ALA:HA	1.05	1.02
1:E:389:MET:HE2	1:E:390:LYS:HD2	1.36	1.02
1:C:215:LEU:HD11	1:C:323:VAL:HB	1.39	1.00
1:D:226:LYS:HD3	1:D:253:ASP:HB3	1.42	1.00
1:G:284:ARG:HH11	1:G:284:ARG:HG3	1.28	0.98
1:A:166:MET:HE1	1:A:403:THR:HG21	1.45	0.98
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.46	0.97
1:G:198:GLY:H	1:G:277:LYS:HE3	1.29	0.97
1:A:383:ALA:HB1	1:A:384:ALA:CA	1.95	0.96
1:G:176:THR:HG22	1:G:378:VAL:HG22	1.46	0.96
1:B:215:LEU:HD22	1:B:246:PRO:HB2	1.46	0.95
1:A:383:ALA:CB	1:A:384:ALA:HA	1.92	0.95
1:G:278:ALA:HB1	1:G:279:PRO:HD2	1.50	0.94
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.49	0.94
1:A:270:ILE:HD13	1:A:273:VAL:HB	1.48	0.93
1:F:301:ILE:HD12	1:F:307:MET:HB3	1.49	0.93
1:F:225:LYS:HD2	1:F:309:LEU:HD11	1.49	0.92
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.48	0.91
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.54	0.90
1:A:218:PRO:HG3	1:A:323:VAL:HG12	1.53	0.89
1:A:183:LEU:HA	1:A:383:ALA:CB	2.00	0.89
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.54	0.89
1:C:222:LEU:HB3	1:C:300:VAL:HG23	1.55	0.89
1:A:266:THR:HA	1:A:270:ILE:CG2	2.03	0.88
1:C:225:LYS:C	1:C:227:ILE:HG13	1.93	0.88
1:G:352:GLN:HA	1:G:355:GLU:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ILE:HD12	1:C:451:LEU:HD13	1.56	0.87
1:C:232:GLU:HB3	1:C:233:MET:CE	2.05	0.87
1:G:222:LEU:HD11	1:G:300:VAL:HA	1.55	0.86
1:F:225:LYS:HG2	1:F:303:GLU:HG3	1.54	0.86
1:G:281:PHE:HB3	1:G:285:ARG:CB	2.06	0.85
5:A:608:MPD:H52	5:A:608:MPD:H11	1.59	0.85
1:B:227:ILE:HG21	1:B:233:MET:HE3	1.57	0.84
1:E:444:LEU:HA	1:E:447:MET:HE3	1.58	0.84
1:C:225:LYS:HA	1:C:227:ILE:HD11	1.57	0.84
1:C:353:ILE:HG12	1:C:365:LEU:HD22	1.60	0.84
1:E:207:LYS:NZ	1:E:210:THR:HG21	1.92	0.83
1:F:77:VAL:HG13	1:F:506:TYR:HB3	1.58	0.83
1:G:383:ALA:HB2	1:G:392:LYS:HD3	1.60	0.83
1:B:259:LEU:HD12	1:B:260:ALA:N	1.92	0.83
1:G:183:LEU:HD12	1:G:384:ALA:HB3	1.59	0.83
1:G:279:PRO:HB2	1:G:285:ARG:HB2	1.60	0.82
1:C:225:LYS:HG2	1:C:253:ASP:O	1.79	0.82
1:F:247:LEU:HD21	1:F:249:ILE:HD11	1.60	0.82
1:C:225:LYS:HA	1:C:227:ILE:CD1	2.10	0.81
1:G:223:ALA:HA	1:G:224:ASP:HB2	1.60	0.81
1:A:39:VAL:HG21	1:B:16:MET:CE	2.11	0.81
1:C:314:LEU:H	1:C:314:LEU:HD12	1.46	0.81
1:C:235:PRO:HG2	1:C:310:GLU:HG2	1.63	0.80
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.63	0.80
1:A:16:MET:HG2	1:A:514:MET:HE3	1.63	0.80
1:G:268:ARG:HG3	1:G:268:ARG:HH11	1.46	0.80
1:F:221:LEU:HD23	1:F:249:ILE:HG23	1.62	0.79
1:G:251:ALA:HB1	1:G:252:GLU:HB2	1.62	0.79
1:B:39:VAL:HG21	1:C:16:MET:HE1	1.65	0.79
1:A:131:LEU:HD13	1:A:422:VAL:HG21	1.63	0.79
1:C:225:LYS:HD2	1:C:227:ILE:HD12	1.64	0.79
1:E:270:ILE:HG22	1:E:271:VAL:H	1.48	0.78
1:F:204:PHE:HB3	1:F:266:THR:CB	2.12	0.78
1:C:284:ARG:HE	1:C:364:LYS:HE2	1.47	0.78
1:G:226:LYS:HB2	1:G:227:ILE:HA	1.66	0.78
1:G:221:LEU:HD11	1:G:247:LEU:HD21	1.65	0.77
1:C:225:LYS:CB	1:C:251:ALA:HB1	2.12	0.77
1:C:314:LEU:O	1:C:317:LEU:HG	1.85	0.77
1:A:183:LEU:HD23	1:A:383:ALA:CB	2.13	0.77
1:A:302:SER:HB2	1:A:305:ILE:HG13	1.66	0.77
1:E:85:ALA:HB1	1:E:499:VAL:HG22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:HG22	1:C:228:SER:H	1.47	0.77
1:G:250:ILE:HG13	1:G:251:ALA:H	1.50	0.77
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.67	0.77
1:D:308:GLU:HB2	1:D:311:LYS:HE3	1.67	0.77
1:G:225:LYS:HB3	1:G:226:LYS:HG2	1.67	0.77
1:F:301:ILE:CD1	1:F:307:MET:HB3	2.14	0.77
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.68	0.76
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.67	0.76
1:C:230:ILE:HG22	1:C:258:ALA:HB1	1.67	0.76
1:G:385:THR:HB	1:G:388:GLU:HB3	1.67	0.76
1:G:281:PHE:CB	1:G:285:ARG:HB3	2.07	0.76
1:E:183:LEU:CD1	1:E:384:ALA:HB2	2.14	0.76
1:C:215:LEU:HD11	1:C:323:VAL:CB	2.16	0.76
1:A:266:THR:HA	1:A:270:ILE:HG21	1.66	0.76
1:A:270:ILE:HG23	1:A:272:LYS:N	2.01	0.76
1:E:207:LYS:HE3	1:E:214:GLU:CG	2.16	0.76
1:E:444:LEU:HD23	1:E:447:MET:HE3	1.68	0.76
1:C:178:GLU:HG2	1:C:322:ARG:NH1	2.01	0.76
1:B:222:LEU:HD23	1:B:250:ILE:HB	1.68	0.76
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.66	0.76
1:A:223:ALA:HA	1:A:301:ILE:HG23	1.66	0.75
1:F:218:PRO:CA	1:F:246:PRO:HG2	2.17	0.75
1:D:215:LEU:HD22	1:D:246:PRO:HB2	1.66	0.75
1:C:230:ILE:HG13	1:C:262:LEU:HD11	1.69	0.75
1:G:198:GLY:N	1:G:277:LYS:HE3	2.02	0.75
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.69	0.74
5:A:606:MPD:H53	5:A:606:MPD:HM2	1.68	0.74
1:E:183:LEU:HD12	1:E:183:LEU:O	1.87	0.74
1:G:185:ASP:OD1	1:G:185:ASP:N	2.20	0.74
1:B:305:ILE:HG23	1:B:307:MET:HG3	1.68	0.74
1:C:199:TYR:OH	1:C:327:LYS:NZ	2.17	0.74
1:G:281:PHE:HB2	1:G:282:GLY:CA	2.19	0.73
1:G:249:ILE:O	1:G:275:ALA:HA	1.88	0.73
1:E:444:LEU:HD23	1:E:447:MET:CE	2.18	0.73
1:A:230:ILE:HD12	1:A:261:THR:CG2	2.13	0.73
1:G:223:ALA:HB3	1:G:252:GLU:H	1.54	0.73
1:C:225:LYS:HD2	1:C:227:ILE:CD1	2.17	0.73
1:E:183:LEU:HD13	1:E:384:ALA:CB	2.18	0.73
1:C:352:GLN:HB2	1:C:365:LEU:HD11	1.68	0.73
1:G:281:PHE:HB2	1:G:282:GLY:HA2	1.70	0.73
1:C:256:GLY:HA3	1:C:259:LEU:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:VAL:O	1:G:267:MET:HG2	1.88	0.73
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.71	0.73
1:A:13:ARG:NH1	7:A:773:HOH:O	2.21	0.73
1:C:350:ARG:HE	1:C:369:VAL:HG21	1.53	0.72
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.71	0.72
1:G:226:LYS:H	1:G:227:ILE:HG13	1.53	0.72
1:F:39:VAL:HG21	1:G:16:MET:CE	2.18	0.72
1:G:248:LEU:CD2	1:G:250:ILE:HG23	2.19	0.72
1:A:248:LEU:HD22	1:A:323:VAL:HG21	1.71	0.72
1:C:284:ARG:NE	1:C:364:LYS:HE2	2.04	0.72
1:C:227:ILE:HG22	1:C:233:MET:CE	2.20	0.72
1:G:222:LEU:HD13	1:G:300:VAL:HG13	1.72	0.72
1:E:82:ASN:ND2	7:E:743:HOH:O	2.23	0.72
1:G:176:THR:CG2	1:G:378:VAL:HG22	2.19	0.71
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.71	0.71
1:C:239:ALA:HB1	1:C:314:LEU:HD21	1.71	0.71
1:G:199:TYR:CE2	1:G:327:LYS:HA	2.25	0.71
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.71	0.71
1:A:266:THR:HA	1:A:270:ILE:HG22	1.72	0.71
1:G:230:ILE:HD12	1:G:234:LEU:HD21	1.73	0.71
1:G:222:LEU:HD22	1:G:300:VAL:HG22	1.73	0.71
1:B:255:GLU:CA	1:B:259:LEU:HD23	2.15	0.71
1:C:230:ILE:CG2	1:C:258:ALA:HB1	2.20	0.71
1:G:383:ALA:HB1	1:G:388:GLU:HG2	1.72	0.71
1:E:169:VAL:HG13	1:E:173:GLY:HA3	1.73	0.71
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.73	0.70
1:A:207:LYS:HG3	1:A:214:GLU:HG3	1.72	0.70
1:G:223:ALA:HB3	1:G:252:GLU:N	2.06	0.70
1:F:218:PRO:HA	1:F:246:PRO:HG2	1.72	0.70
1:C:349:ILE:O	1:C:365:LEU:HD21	1.90	0.70
1:E:222:LEU:HD13	1:E:293:ALA:HB2	1.73	0.70
1:C:232:GLU:HG2	1:C:310:GLU:OE2	1.91	0.70
1:B:177:VAL:HG11	1:B:397:GLU:HG3	1.72	0.70
1:D:226:LYS:CD	1:D:253:ASP:HB3	2.18	0.70
1:C:420:ILE:CD1	1:C:451:LEU:HD13	2.22	0.70
1:B:181:THR:HG22	1:B:182:GLY:H	1.56	0.70
1:A:304:GLU:OE1	1:A:304:GLU:N	2.25	0.70
1:C:276:VAL:HG11	1:C:325:ILE:HD13	1.73	0.70
1:C:310:GLU:N	1:C:310:GLU:OE1	2.24	0.69
1:C:252:GLU:OE2	1:C:285:ARG:NH2	2.25	0.69
1:F:359:ASP:OD1	1:F:362:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ILE:HD12	1:C:326:ASN:H	1.57	0.69
1:G:225:LYS:HB3	1:G:226:LYS:CG	2.22	0.69
1:D:265:ASN:HB3	1:D:270:ILE:HG23	1.72	0.69
1:G:183:LEU:CD1	1:G:384:ALA:HB3	2.22	0.69
1:B:248:LEU:HD22	1:B:323:VAL:HG11	1.75	0.69
1:F:383:ALA:HB1	1:F:388:GLU:HB3	1.75	0.69
1:G:268:ARG:NH1	1:G:270:ILE:HB	2.06	0.69
1:G:217:SER:N	1:G:218:PRO:HD3	2.07	0.69
1:G:282:GLY:O	1:G:285:ARG:NH1	2.24	0.69
1:G:222:LEU:CD1	1:G:300:VAL:HA	2.22	0.69
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.08	0.69
1:B:18:ARG:HD2	7:B:781:HOH:O	1.92	0.69
1:F:204:PHE:HB3	1:F:266:THR:HG21	1.72	0.69
1:B:232:GLU:HA	1:B:310:GLU:HG2	1.75	0.69
1:A:226:LYS:HD2	1:A:226:LYS:H	1.58	0.69
1:F:233:MET:HG2	1:F:309:LEU:HD23	1.75	0.68
1:F:239:ALA:HB1	1:F:314:LEU:HD21	1.75	0.68
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.76	0.68
1:D:194:GLN:O	1:D:371:LYS:HE3	1.93	0.68
1:A:373:ALA:HA	5:A:604:MPD:H52	1.74	0.68
1:C:213:VAL:HG22	1:C:325:ILE:HG23	1.76	0.68
1:F:246:PRO:HB3	1:F:272:LYS:HE3	1.76	0.68
1:G:268:ARG:HH12	1:G:271:VAL:HG23	1.59	0.68
1:G:223:ALA:HB1	1:G:224:ASP:C	2.14	0.68
1:A:183:LEU:HD23	1:A:383:ALA:HB1	1.75	0.68
1:G:230:ILE:HG12	1:G:257:GLU:OE1	1.94	0.68
1:B:39:VAL:HG12	1:C:69:MET:CE	2.24	0.68
1:F:284:ARG:O	1:F:288:MET:HG2	1.94	0.67
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.75	0.67
1:D:231:ARG:HA	1:D:234:LEU:HD12	1.76	0.67
5:A:606:MPD:HM1	1:G:456:LEU:HG	1.77	0.67
1:G:250:ILE:HA	1:G:276:VAL:HG22	1.77	0.67
1:A:39:VAL:HG21	1:B:16:MET:HE1	1.75	0.67
1:C:198:GLY:O	1:C:276:VAL:HG12	1.95	0.67
1:G:221:LEU:HD23	1:G:317:LEU:HG	1.75	0.67
1:B:313:THR:HG22	1:B:314:LEU:H	1.58	0.67
1:G:173:GLY:O	1:G:404:ARG:NH2	2.28	0.67
1:A:218:PRO:HG3	1:A:323:VAL:CG1	2.24	0.67
1:D:303:GLU:OE1	1:D:303:GLU:N	2.28	0.67
1:G:310:GLU:OE1	1:G:310:GLU:N	2.28	0.66
1:C:361:ASP:HA	1:C:364:LYS:HE3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:606:MPD:CM	1:G:456:LEU:HG	2.25	0.66
1:A:270:ILE:N	1:A:271:VAL:HA	2.11	0.66
1:A:350:ARG:HA	1:A:353:ILE:HD12	1.78	0.66
1:G:251:ALA:HB3	1:G:289:LEU:HD21	1.75	0.66
1:C:353:ILE:HG12	1:C:365:LEU:CD2	2.26	0.66
1:A:518:GLU:HG2	7:G:730:HOH:O	1.96	0.66
1:F:268:ARG:HA	1:F:268:ARG:HE	1.60	0.66
1:G:197:ALA:HB3	1:G:330:THR:CG2	2.25	0.66
1:A:144:ILE:HG21	1:A:166:MET:HE3	1.76	0.66
1:F:235:PRO:CG	1:F:310:GLU:HA	2.26	0.66
1:C:259:LEU:HA	1:C:262:LEU:HD13	1.78	0.66
1:C:263:VAL:O	1:C:266:THR:HG22	1.94	0.66
1:D:209:GLU:HG2	1:D:210:THR:H	1.61	0.66
1:A:183:LEU:CA	1:A:383:ALA:HB2	2.09	0.65
1:C:235:PRO:HG2	1:C:310:GLU:CG	2.26	0.65
1:F:268:ARG:HA	1:F:268:ARG:NE	2.10	0.65
1:D:187:LEU:HD23	1:D:379:ILE:HG12	1.77	0.65
1:C:199:TYR:CE1	1:C:202:PRO:HA	2.31	0.65
1:F:199:TYR:CE1	1:F:202:PRO:HA	2.32	0.65
1:F:386:GLU:HG2	1:F:390:LYS:NZ	2.11	0.65
1:G:287:ALA:HB1	1:G:368:ARG:NH1	2.12	0.65
1:G:224:ASP:CG	1:G:302:SER:HB2	2.17	0.65
1:E:207:LYS:HZ3	1:E:210:THR:HG21	1.60	0.65
1:A:381:VAL:HG11	1:A:392:LYS:HB3	1.79	0.65
1:G:261:THR:HA	1:G:264:VAL:CG1	2.27	0.65
1:G:268:ARG:NH1	1:G:268:ARG:HG3	2.09	0.65
1:F:131:LEU:HD21	1:F:500:THR:HG22	1.79	0.65
1:D:30:THR:HB	1:D:51:LYS:O	1.97	0.65
1:G:250:ILE:CA	1:G:276:VAL:HG22	2.27	0.64
1:C:252:GLU:O	1:C:277:LYS:HG3	1.96	0.64
1:E:68:ASN:O	1:E:72:GLN:HG2	1.96	0.64
1:A:242:LYS:NZ	1:B:229:ASN:HB2	2.13	0.64
1:F:183:LEU:HD13	1:F:184:GLN:HG2	1.78	0.64
1:G:207:LYS:HB3	1:G:209:GLU:OE2	1.98	0.64
1:A:384:ALA:HB3	1:A:388:GLU:OE1	1.97	0.64
1:G:222:LEU:HD11	1:G:301:ILE:H	1.61	0.64
1:B:319:GLN:HB2	1:B:336:VAL:HG21	1.79	0.64
1:F:234:LEU:N	1:F:235:PRO:HD2	2.12	0.64
1:F:204:PHE:HB3	1:F:266:THR:CG2	2.26	0.64
1:C:325:ILE:CD1	1:C:326:ASN:H	2.11	0.64
1:A:220:ILE:HD12	1:A:296:THR:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:CD1	1:C:317:LEU:HD11	2.33	0.64
1:A:10:ASN:HB3	7:A:740:HOH:O	1.97	0.64
1:D:228:SER:O	1:D:258:ALA:N	2.29	0.64
1:C:215:LEU:HD22	1:C:218:PRO:HB3	1.78	0.63
1:G:367:GLU:O	1:G:371:LYS:HG2	1.98	0.63
1:E:301:ILE:HG21	1:E:309:LEU:HD23	1.79	0.63
1:F:301:ILE:HD11	1:F:308:GLU:N	2.13	0.63
1:E:266:THR:OG1	1:E:273:VAL:HG12	1.98	0.63
1:C:227:ILE:HG22	1:C:233:MET:HE1	1.80	0.63
1:A:104:LEU:HB3	5:A:605:MPD:HM1	1.81	0.63
1:G:284:ARG:CG	1:G:284:ARG:HH11	2.07	0.63
1:G:301:ILE:HG23	1:G:307:MET:HG3	1.80	0.63
1:F:39:VAL:HG21	1:G:16:MET:HE1	1.79	0.63
1:D:225:LYS:HD2	1:D:303:GLU:HG2	1.80	0.63
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.80	0.63
1:B:209:GLU:HG2	1:B:210:THR:N	2.14	0.63
1:F:358:SER:HB3	1:F:361:ASP:HB2	1.80	0.63
1:G:278:ALA:CB	1:G:279:PRO:HD2	2.20	0.63
1:F:221:LEU:HB3	1:F:249:ILE:HD12	1.79	0.63
1:E:247:LEU:HB3	1:E:273:VAL:HG23	1.80	0.63
1:B:513:LEU:O	1:B:517:THR:HG23	1.98	0.63
1:E:445:ARG:NH1	5:E:604:MPD:HM1	2.14	0.63
1:C:215:LEU:HD13	1:C:218:PRO:CG	2.28	0.63
1:G:222:LEU:CD2	1:G:300:VAL:HG22	2.29	0.63
1:D:160:LYS:NZ	1:D:164:GLU:OE2	2.23	0.63
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.80	0.63
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.98	0.62
1:B:229:ASN:ND2	1:B:231:ARG:HB2	2.13	0.62
1:E:215:LEU:HB2	1:E:323:VAL:CG2	2.29	0.62
1:D:165:ALA:O	1:D:169:VAL:HG22	1.99	0.62
1:A:310:GLU:N	1:A:310:GLU:OE1	2.32	0.62
1:F:319:GLN:HB2	1:F:336:VAL:HG21	1.79	0.62
1:B:194:GLN:O	1:B:371:LYS:HE3	2.00	0.62
1:F:213:VAL:HG12	1:F:214:GLU:H	1.65	0.62
1:E:39:VAL:HG21	1:F:16:MET:CE	2.30	0.62
1:F:248:LEU:HD13	1:F:325:ILE:HD11	1.81	0.62
1:D:463:SER:HB2	7:D:740:HOH:O	1.99	0.62
1:E:207:LYS:HE3	1:E:214:GLU:HG3	1.82	0.62
1:F:179:ASP:HB3	1:F:389:MET:SD	2.40	0.62
1:C:229:ASN:OD1	1:C:230:ILE:N	2.30	0.61
1:C:359:ASP:OD1	1:C:362:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ILE:HD11	1:G:493:ILE:HA	1.82	0.61
1:G:319:GLN:HB3	1:G:336:VAL:CG2	2.29	0.61
1:D:400:LEU:O	1:D:404:ARG:HG2	2.00	0.61
1:G:279:PRO:CB	1:G:285:ARG:HB2	2.30	0.61
1:A:284:ARG:HD3	1:A:364:LYS:NZ	2.15	0.61
1:C:346:VAL:O	1:C:350:ARG:HG2	2.00	0.61
1:A:302:SER:HB2	1:A:305:ILE:CG1	2.30	0.61
1:G:218:PRO:HG2	1:G:323:VAL:HG22	1.81	0.61
1:G:291:ASP:HB3	1:G:372:LEU:HD11	1.81	0.61
1:G:392:LYS:NZ	7:G:737:HOH:O	2.34	0.61
1:F:231:ARG:HG3	1:F:231:ARG:HH11	1.65	0.61
1:B:198:GLY:H	1:B:277:LYS:HE3	1.66	0.61
1:G:261:THR:O	1:G:264:VAL:HG13	2.01	0.61
1:E:310:GLU:OE1	1:E:310:GLU:N	2.32	0.61
1:F:498:LYS:HG3	1:F:501:ARG:NH2	2.16	0.61
1:C:225:LYS:CA	1:C:227:ILE:HG13	2.30	0.61
1:C:200:LEU:HD12	1:C:254:VAL:CG2	2.31	0.61
1:D:308:GLU:O	1:D:311:LYS:HG2	1.99	0.61
1:F:217:SER:HA	1:F:320:ALA:O	2.01	0.61
1:B:181:THR:HG22	1:B:182:GLY:N	2.15	0.60
1:F:221:LEU:HB3	1:F:249:ILE:CD1	2.32	0.60
1:C:225:LYS:HA	1:C:227:ILE:CG1	2.31	0.60
1:F:247:LEU:CD2	1:F:249:ILE:HD11	2.32	0.60
1:F:348:GLN:O	1:F:352:GLN:HG3	2.02	0.60
1:F:496:PRO:HB2	1:F:499:VAL:HG13	1.84	0.60
1:D:385:THR:CG2	1:D:388:GLU:HG2	2.30	0.60
1:G:197:ALA:HA	1:G:277:LYS:HG2	1.84	0.60
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.67	0.60
1:D:315:GLU:N	1:D:315:GLU:OE1	2.34	0.60
1:C:227:ILE:CG2	1:C:233:MET:CE	2.80	0.60
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.84	0.60
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.83	0.60
1:G:222:LEU:HD21	1:G:300:VAL:HA	1.83	0.60
1:A:34:LYS:HG3	1:A:458:CYS:SG	2.42	0.60
1:G:284:ARG:NH1	1:G:284:ARG:HG3	2.08	0.59
1:E:253:ASP:OD1	1:E:254:VAL:N	2.35	0.59
1:B:268:ARG:NH1	1:B:268:ARG:HG2	2.18	0.59
1:C:215:LEU:CD1	1:C:323:VAL:HB	2.24	0.59
1:A:270:ILE:HG23	1:A:271:VAL:C	2.22	0.59
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.83	0.59
1:E:207:LYS:HZ2	1:E:210:THR:HG21	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:LEU:HD13	1:G:254:VAL:HG22	1.85	0.59
1:F:227:ILE:HD12	1:F:309:LEU:HD21	1.83	0.59
1:D:179:ASP:HA	1:D:389:MET:HE1	1.83	0.59
1:G:221:LEU:HG	1:G:247:LEU:HD11	1.84	0.59
1:A:16:MET:CG	1:A:514:MET:HE3	2.32	0.59
1:G:276:VAL:HG23	1:G:278:ALA:H	1.67	0.59
1:C:213:VAL:HG22	1:C:325:ILE:CG2	2.33	0.59
1:F:149:THR:HG21	1:F:156:GLU:HG2	1.84	0.59
1:G:221:LEU:CD2	1:G:317:LEU:HG	2.33	0.59
1:C:253:ASP:OD1	1:C:254:VAL:N	2.35	0.59
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.32	0.59
1:G:30:THR:HB	1:G:51:LYS:O	2.03	0.59
1:E:39:VAL:HG21	1:F:16:MET:HE1	1.84	0.59
1:B:264:VAL:O	1:B:268:ARG:HG3	2.03	0.59
1:G:250:ILE:HG13	1:G:251:ALA:N	2.15	0.59
1:D:200:LEU:HD12	1:D:254:VAL:HB	1.84	0.59
1:B:39:VAL:HG21	1:C:16:MET:CE	2.31	0.59
1:E:235:PRO:CG	1:E:310:GLU:HA	2.32	0.59
1:F:183:LEU:HD12	1:F:184:GLN:H	1.67	0.59
1:A:198:GLY:HA3	1:A:327:LYS:O	2.03	0.59
1:B:420:ILE:HD13	1:B:448:GLU:HG2	1.85	0.59
1:G:301:ILE:HG12	1:G:307:MET:HG2	1.85	0.58
1:D:308:GLU:CB	1:D:311:LYS:HE3	2.33	0.58
1:A:242:LYS:CE	1:B:229:ASN:HB2	2.33	0.58
1:G:154:SER:HB3	7:G:716:HOH:O	2.03	0.58
1:E:194:GLN:O	1:E:371:LYS:HE3	2.03	0.58
1:G:281:PHE:HD2	1:G:282:GLY:HA2	1.66	0.58
1:G:346:VAL:O	1:G:350:ARG:HG3	2.03	0.58
5:G:604:MPD:H51	7:G:748:HOH:O	2.04	0.58
1:A:282:GLY:O	1:A:286:LYS:HG2	2.03	0.58
1:C:192:GLY:HA2	1:C:295:LEU:HD21	1.86	0.58
1:G:197:ALA:HB3	1:G:330:THR:HG21	1.85	0.58
1:F:213:VAL:HG12	1:F:214:GLU:N	2.18	0.58
1:C:16:MET:HG3	1:C:520:MET:HE1	1.85	0.58
1:A:284:ARG:CZ	1:A:364:LYS:HG2	2.34	0.58
1:D:149:THR:O	1:D:154:SER:N	2.35	0.58
1:E:389:MET:CE	1:E:390:LYS:HD2	2.22	0.58
1:C:353:ILE:CG1	1:C:365:LEU:HD22	2.33	0.58
1:B:178:GLU:HA	1:B:393:LYS:HE3	1.86	0.58
1:C:200:LEU:CD1	1:C:254:VAL:HG23	2.34	0.58
1:C:358:SER:OG	1:C:361:ASP:OD2	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:ASN:O	1:F:269:GLY:N	2.35	0.58
1:F:319:GLN:HB2	1:F:336:VAL:CG2	2.34	0.58
1:E:197:ALA:HB1	1:E:276:VAL:HB	1.85	0.58
1:E:205:ILE:HD12	1:E:211:GLY:HA2	1.85	0.58
1:D:235:PRO:HG2	1:D:310:GLU:HA	1.85	0.58
1:C:10:ASN:O	1:C:14:VAL:HG23	2.04	0.58
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.86	0.58
1:C:179:ASP:HB3	1:C:389:MET:CE	2.33	0.58
1:F:366:GLN:HA	1:F:369:VAL:HG22	1.85	0.58
1:G:361:ASP:O	1:G:365:LEU:HG	2.04	0.58
7:C:733:HOH:O	1:D:518:GLU:HG2	2.02	0.58
1:G:248:LEU:HD21	1:G:250:ILE:HG23	1.85	0.57
1:A:183:LEU:HD23	1:A:383:ALA:HB2	1.83	0.57
1:C:215:LEU:HD13	1:C:218:PRO:HD3	1.85	0.57
1:C:325:ILE:HD13	1:C:330:THR:OG1	2.03	0.57
1:D:225:LYS:HB2	1:D:303:GLU:CD	2.25	0.57
1:E:204:PHE:HB3	1:E:266:THR:HG21	1.86	0.57
1:A:420:ILE:HD13	1:A:448:GLU:HG2	1.86	0.57
1:F:250:ILE:HG22	1:F:289:LEU:HD21	1.85	0.57
1:B:347:ALA:O	1:B:351:GLN:HG2	2.04	0.57
1:G:299:THR:HB	1:G:316:ASP:OD1	2.04	0.57
1:A:302:SER:HB2	1:A:305:ILE:CD1	2.34	0.57
1:D:178:GLU:O	1:D:381:VAL:HG23	2.04	0.57
1:A:285:ARG:O	1:A:289:LEU:HG	2.04	0.57
1:C:265:ASN:O	1:C:270:ILE:HG12	2.05	0.57
1:G:234:LEU:N	1:G:235:PRO:HD2	2.19	0.57
1:G:271:VAL:CG1	1:G:273:VAL:HG23	2.35	0.57
1:D:388:GLU:O	1:D:392:LYS:N	2.31	0.57
1:A:287:ALA:HB1	1:A:368:ARG:NH1	2.19	0.57
1:G:230:ILE:CG2	1:G:258:ALA:HA	2.35	0.57
1:D:136:VAL:HG13	1:D:137:PRO:HD2	1.85	0.57
1:G:226:LYS:N	1:G:227:ILE:HG13	2.18	0.57
1:C:215:LEU:CD1	1:C:218:PRO:HG3	2.34	0.57
1:G:215:LEU:HB2	1:G:218:PRO:CG	2.35	0.57
1:G:187:LEU:HD13	1:G:379:ILE:CG2	2.35	0.57
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.86	0.57
1:B:209:GLU:HG2	1:B:210:THR:H	1.70	0.56
1:B:169:VAL:HG23	1:B:173:GLY:HA3	1.87	0.56
1:C:261:THR:HA	1:C:264:VAL:HG12	1.87	0.56
1:F:136:VAL:HG13	1:F:137:PRO:HD2	1.86	0.56
1:C:251:ALA:O	1:C:278:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:CD2	1:B:272:LYS:HG3	2.36	0.56
1:C:69:MET:O	1:C:73:MET:HG3	2.05	0.56
1:C:401:HIS:HB2	7:C:760:HOH:O	2.05	0.56
1:B:86:GLY:HA2	5:B:608:MPD:H12	1.86	0.56
1:C:215:LEU:O	1:C:215:LEU:HD12	2.05	0.56
1:F:218:PRO:CB	1:F:246:PRO:HG2	2.35	0.56
1:F:242:LYS:HG2	1:G:257:GLU:HB2	1.86	0.56
1:E:89:THR:HB	7:E:743:HOH:O	2.05	0.56
1:D:225:LYS:HB2	1:D:303:GLU:CG	2.36	0.56
1:D:209:GLU:N	1:D:209:GLU:OE1	2.27	0.56
1:A:220:ILE:CD1	1:A:296:THR:HG21	2.35	0.56
1:G:395:ARG:HG3	1:G:396:VAL:N	2.21	0.56
1:B:73:MET:HE1	1:B:514:MET:HG2	1.88	0.56
1:D:225:LYS:HB2	1:D:303:GLU:HG2	1.87	0.56
1:G:199:TYR:HE1	1:G:202:PRO:HG3	1.71	0.56
1:G:257:GLU:HG2	1:G:261:THR:HB	1.86	0.56
1:E:270:ILE:HG22	1:E:271:VAL:N	2.18	0.56
1:E:7:LYS:HG2	1:E:66:PHE:CZ	2.41	0.56
1:D:243:ALA:O	1:E:231:ARG:NH1	2.38	0.56
1:C:317:LEU:O	1:C:317:LEU:HD12	2.06	0.56
1:B:277:LYS:HD2	1:B:277:LYS:O	2.06	0.56
1:D:238:GLU:O	1:D:242:LYS:HD3	2.05	0.56
1:D:152:ALA:HB3	1:D:153:ASN:C	2.27	0.56
1:F:381:VAL:HG21	1:F:392:LYS:HG2	1.87	0.56
1:G:257:GLU:HG2	1:G:261:THR:CB	2.36	0.56
1:G:281:PHE:CB	1:G:285:ARG:HD3	2.36	0.55
1:C:325:ILE:HD12	1:C:329:THR:O	2.06	0.55
1:F:498:LYS:HG3	1:F:501:ARG:HH21	1.70	0.55
1:B:214:GLU:OE1	1:B:322:ARG:NH2	2.38	0.55
1:F:177:VAL:CG1	1:F:397:GLU:HG2	2.36	0.55
1:G:281:PHE:CD2	1:G:282:GLY:HA2	2.40	0.55
1:F:204:PHE:CB	1:F:266:THR:HG21	2.37	0.55
1:B:234:LEU:HA	1:B:237:LEU:HD12	1.87	0.55
1:F:225:LYS:HD2	1:F:309:LEU:CD1	2.30	0.55
1:G:265:ASN:HA	1:G:268:ARG:HG2	1.87	0.55
1:E:445:ARG:HH12	5:E:604:MPD:HM1	1.70	0.55
1:A:37:ASN:HB2	1:B:517:THR:HG22	1.88	0.55
1:B:68:ASN:O	1:B:72:GLN:HG2	2.06	0.55
1:C:230:ILE:HG22	1:C:258:ALA:CB	2.35	0.55
1:F:215:LEU:HB2	1:F:323:VAL:CG2	2.29	0.55
7:A:751:HOH:O	1:B:518:GLU:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:VAL:HG13	1:C:506:TYR:HB3	1.89	0.55
1:E:193:MET:HG2	1:E:295:LEU:CD2	2.37	0.55
1:A:401:HIS:HB3	5:A:609:MPD:HM3	1.88	0.55
1:G:152:ALA:HB1	1:G:158:VAL:HG11	1.88	0.55
1:B:276:VAL:CG1	1:B:325:ILE:HD13	2.36	0.55
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.07	0.55
1:D:128:VAL:HG12	1:D:132:LYS:HE3	1.89	0.55
1:C:260:ALA:O	1:C:263:VAL:HG13	2.07	0.55
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.89	0.55
1:F:160:LYS:HE2	1:F:164:GLU:OE2	2.06	0.55
1:G:221:LEU:HD12	1:G:249:ILE:HG12	1.88	0.55
1:B:178:GLU:HB2	1:B:322:ARG:NH1	2.22	0.55
1:E:7:LYS:HD2	1:E:11:ASP:OD1	2.07	0.55
1:B:392:LYS:HE3	7:B:806:HOH:O	2.06	0.55
1:C:213:VAL:HG13	1:C:325:ILE:HG23	1.88	0.54
1:G:205:ILE:HG23	1:G:212:ALA:O	2.06	0.54
1:F:342:ILE:O	1:F:346:VAL:HG23	2.07	0.54
1:C:150:ILE:HB	7:C:787:HOH:O	2.07	0.54
1:A:193:MET:HG3	1:A:371:LYS:HB3	1.89	0.54
1:G:85:ALA:HB1	1:G:499:VAL:HG22	1.89	0.54
1:G:365:LEU:HD12	1:G:366:GLN:N	2.22	0.54
1:C:294:THR:HG23	1:C:341:ALA:HB1	1.87	0.54
1:G:281:PHE:HB2	1:G:282:GLY:O	2.08	0.54
1:A:179:ASP:OD1	1:A:393:LYS:HD2	2.08	0.54
1:G:209:GLU:HG2	1:G:210:THR:N	2.22	0.54
1:B:10:ASN:O	1:B:14:VAL:HG13	2.07	0.54
1:G:229:ASN:ND2	1:G:231:ARG:HB2	2.21	0.54
1:G:278:ALA:HB1	1:G:279:PRO:CD	2.33	0.54
1:A:263:VAL:O	1:A:266:THR:OG1	2.25	0.54
1:G:218:PRO:HG2	1:G:323:VAL:CG2	2.37	0.54
1:F:248:LEU:CD1	1:F:325:ILE:HD11	2.38	0.54
1:B:525:PRO:HD3	7:B:759:HOH:O	2.07	0.54
1:D:260:ALA:O	1:D:264:VAL:HG23	2.06	0.54
1:C:215:LEU:HD13	1:C:218:PRO:CD	2.38	0.54
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.90	0.54
7:D:754:HOH:O	1:E:518:GLU:HG2	2.06	0.54
1:G:279:PRO:HB2	1:G:285:ARG:CB	2.33	0.54
1:A:162:ILE:HG22	1:A:166:MET:CE	2.37	0.54
1:F:232:GLU:CD	1:F:309:LEU:HD13	2.28	0.54
1:F:200:LEU:HD12	1:F:254:VAL:HB	1.89	0.54
1:A:267:MET:HB2	1:A:268:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:HE2	1:C:118[A]:ARG:NH2	2.22	0.54
1:G:200:LEU:HD12	1:G:275:ALA:HB1	1.89	0.54
1:B:441:LYS:HE2	7:B:812:HOH:O	2.08	0.54
1:C:215:LEU:HD13	1:C:218:PRO:HG3	1.90	0.54
1:A:177:VAL:HG11	1:A:397:GLU:HG3	1.89	0.54
1:F:445[B]:ARG:NH2	7:F:720:HOH:O	2.40	0.54
1:C:225:LYS:HA	1:C:227:ILE:HG13	1.89	0.54
1:F:173:GLY:O	1:F:404:ARG:NH2	2.41	0.54
1:A:200:LEU:CD1	1:A:254:VAL:HB	2.38	0.54
1:D:463:SER:O	1:D:467:ASN:HB2	2.08	0.54
1:D:310:GLU:OE1	1:D:310:GLU:N	2.30	0.54
1:C:82:ASN:HB2	1:C:89:THR:OG1	2.08	0.54
1:C:39:VAL:HG12	1:D:69:MET:CE	2.38	0.54
1:G:384:ALA:O	1:G:385:THR:OG1	2.24	0.53
1:C:325:ILE:HG13	1:C:326:ASN:N	2.23	0.53
1:C:305:ILE:CG2	1:C:307:MET:HG3	2.38	0.53
1:E:203:TYR:O	1:E:267:MET:HE2	2.07	0.53
1:F:302:SER:O	1:F:307:MET:HB2	2.08	0.53
1:C:199:TYR:HE1	1:C:202:PRO:HA	1.70	0.53
1:F:288:MET:O	1:F:292:ILE:HG13	2.08	0.53
1:C:385:THR:HG22	1:C:386:GLU:N	2.23	0.53
1:F:30:THR:HB	1:F:51:LYS:O	2.08	0.53
1:A:184:GLN:OE1	1:A:184:GLN:N	2.32	0.53
1:G:281:PHE:HB2	1:G:282:GLY:C	2.29	0.53
1:D:306:GLY:O	1:D:311:LYS:NZ	2.41	0.53
1:F:414:GLY:O	1:F:417:VAL:HG13	2.08	0.53
1:B:229:ASN:HD21	1:B:231:ARG:HB2	1.73	0.53
1:E:383:ALA:HB1	1:E:388:GLU:HB2	1.91	0.53
1:E:232:GLU:HG2	1:E:310:GLU:OE2	2.07	0.53
1:C:120:ILE:O	1:C:124:VAL:HG23	2.07	0.53
1:A:223:ALA:HB3	1:A:251:ALA:HB2	1.89	0.53
1:C:213:VAL:CG2	1:C:325:ILE:HG23	2.38	0.53
1:D:152:ALA:HB3	1:D:155:ASP:H	1.72	0.53
1:B:14:VAL:HG12	5:B:604:MPD:H51	1.90	0.53
1:G:224:ASP:OD2	1:G:302:SER:HB2	2.08	0.53
1:G:221:LEU:HB2	1:G:249:ILE:HG23	1.91	0.53
1:D:265:ASN:HB3	1:D:270:ILE:CG2	2.37	0.53
1:F:281:PHE:CA	1:F:285:ARG:HB2	2.39	0.53
1:A:136:VAL:HG13	1:A:137:PRO:HD2	1.89	0.53
1:F:231:ARG:HD2	1:F:231:ARG:O	2.08	0.53
1:B:14:VAL:HG12	5:B:604:MPD:C5	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ASP:OD1	1:B:362:ARG:HD2	2.08	0.53
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.09	0.53
1:F:310:GLU:OE1	1:F:310:GLU:N	2.33	0.53
1:G:303:GLU:OE2	1:G:308:GLU:HA	2.08	0.53
1:F:221:LEU:HA	1:F:317:LEU:HD23	1.90	0.53
1:D:193:MET:CE	1:D:371:LYS:HD3	2.39	0.53
1:G:187:LEU:HD13	1:G:379:ILE:HG23	1.91	0.53
1:C:276:VAL:HG11	1:C:325:ILE:CD1	2.37	0.52
1:B:86:GLY:CA	5:B:608:MPD:H12	2.40	0.52
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.91	0.52
1:G:326:ASN:HB2	1:G:329:THR:HG23	1.91	0.52
1:B:217:SER:HB3	1:B:245:LYS:NZ	2.24	0.52
1:C:243:ALA:HB3	1:C:244:GLY:CA	2.39	0.52
1:A:381:VAL:HG21	1:A:393:LYS:CA	2.37	0.52
1:C:281:PHE:HA	1:C:285:ARG:HD3	1.91	0.52
1:B:111:MET:HG2	1:B:435:ASP:OD1	2.10	0.52
1:C:194:GLN:OE1	1:C:331:THR:OG1	2.27	0.52
1:A:77:VAL:HG13	1:A:506:TYR:HB3	1.91	0.52
1:E:2:ALA:HB3	7:E:751:HOH:O	2.08	0.52
1:B:263:VAL:HG22	1:B:267:MET:CE	2.40	0.52
1:G:273:VAL:HG12	1:G:274:ALA:N	2.23	0.52
1:B:177:VAL:CG1	1:B:397:GLU:HG3	2.39	0.52
1:B:301:ILE:HD13	1:B:312:ALA:HB2	1.91	0.52
1:D:230:ILE:HG21	1:D:261:THR:HG21	1.91	0.52
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.91	0.52
1:G:171:LYS:HD3	1:G:407:VAL:HG13	1.91	0.52
1:D:236:VAL:O	1:D:240:VAL:HG23	2.10	0.52
1:C:227:ILE:HG22	1:C:233:MET:HE3	1.92	0.52
1:B:16:MET:HE2	1:B:73:MET:SD	2.50	0.52
1:A:169:VAL:CG1	1:A:173:GLY:HA3	2.40	0.52
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.90	0.52
1:C:259:LEU:CA	1:C:262:LEU:HD13	2.40	0.52
1:C:248:LEU:CD2	1:C:323:VAL:HG11	2.37	0.52
1:F:179:ASP:HB3	1:F:389:MET:CE	2.40	0.52
1:G:152:ALA:HB1	1:G:158:VAL:CG1	2.39	0.52
1:G:326:ASN:N	1:G:329:THR:O	2.38	0.52
1:B:111:MET:HE2	7:B:802:HOH:O	2.08	0.52
1:B:160:LYS:HE2	1:B:164:GLU:OE2	2.09	0.52
1:G:227:ILE:HD12	1:G:227:ILE:N	2.24	0.52
1:G:171:LYS:HD3	1:G:407:VAL:CG1	2.39	0.52
1:F:10:ASN:O	1:F:14:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLY:O	1:B:259:LEU:HG	2.09	0.52
1:C:229:ASN:HA	1:C:259:LEU:HD11	1.91	0.52
1:C:270:ILE:HG13	1:C:271:VAL:N	2.25	0.52
1:C:489:ILE:CD1	1:C:494:LEU:HD22	2.39	0.52
1:E:319:GLN:HG3	1:E:336:VAL:HG21	1.90	0.52
1:A:236:VAL:O	1:A:240:VAL:HG23	2.10	0.52
1:C:222:LEU:CB	1:C:300:VAL:HG23	2.35	0.52
1:G:222:LEU:O	1:G:222:LEU:HD12	2.09	0.52
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.92	0.52
1:D:38:VAL:HG22	1:E:519:CYS:HB3	1.92	0.52
1:C:417:VAL:HG21	1:C:488:MET:HG3	1.92	0.52
1:G:197:ALA:HA	1:G:277:LYS:CG	2.40	0.51
1:A:271:VAL:HG23	1:A:272:LYS:HD3	1.91	0.51
1:G:193:MET:HB2	1:G:371:LYS:HB3	1.92	0.51
1:B:30:THR:HB	1:B:51:LYS:O	2.09	0.51
1:C:221:LEU:HD13	1:C:222:LEU:N	2.25	0.51
1:C:346:VAL:HG13	1:C:369:VAL:HG23	1.91	0.51
1:C:342:ILE:O	1:C:346:VAL:HG23	2.09	0.51
1:A:397:GLU:O	1:A:401:HIS:ND1	2.32	0.51
1:G:285:ARG:HG2	1:G:286:LYS:N	2.24	0.51
1:C:256:GLY:CA	1:C:259:LEU:HB2	2.39	0.51
1:C:194:GLN:O	1:C:371:LYS:HE3	2.09	0.51
1:A:327:LYS:HG3	1:A:328:ASP:OD2	2.10	0.51
1:B:308:GLU:CG	1:B:311:LYS:HE2	2.39	0.51
1:B:77:VAL:HG21	1:B:510:VAL:HB	1.92	0.51
1:G:197:ALA:HB3	1:G:330:THR:HG22	1.91	0.51
1:F:265:ASN:HA	1:F:268:ARG:HB2	1.93	0.51
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.10	0.51
1:E:193:MET:CE	1:E:372:LEU:HD12	2.40	0.51
1:C:489:ILE:HD13	1:C:494:LEU:HD22	1.93	0.51
1:E:279:PRO:HG2	1:E:288:MET:HG2	1.91	0.51
1:G:268:ARG:NH1	1:G:271:VAL:HG23	2.26	0.51
1:F:200:LEU:HD21	1:F:277:LYS:HB2	1.93	0.51
1:G:260:ALA:O	1:G:263:VAL:HG12	2.10	0.51
1:A:39:VAL:HG21	1:B:16:MET:HE3	1.88	0.51
1:D:152:ALA:N	1:D:153:ASN:HA	2.25	0.51
1:C:150:ILE:HD11	1:C:493:ILE:HA	1.92	0.51
1:C:82:ASN:ND2	7:C:737:HOH:O	2.43	0.51
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.92	0.51
1:F:209:GLU:HG2	1:F:210:THR:HG23	1.93	0.51
1:G:230:ILE:HG22	1:G:258:ALA:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ILE:CG1	1:C:326:ASN:H	2.24	0.51
1:B:253:ASP:OD1	1:B:254:VAL:N	2.42	0.51
1:G:150:ILE:CD1	1:G:493:ILE:HA	2.41	0.50
1:C:112:ASN:HB3	1:C:115:ASP:HB2	1.93	0.50
1:G:251:ALA:HB2	1:G:279:PRO:HD2	1.92	0.50
1:C:344:GLY:O	1:C:348:GLN:HG3	2.11	0.50
1:G:268:ARG:CG	1:G:268:ARG:HH11	2.22	0.50
1:G:120:ILE:O	1:G:124:VAL:HG23	2.11	0.50
1:C:314:LEU:CD1	1:C:314:LEU:H	2.21	0.50
1:E:204:PHE:O	1:E:213:VAL:HG22	2.11	0.50
1:C:364:LYS:HG3	1:C:365:LEU:N	2.27	0.50
1:B:458:CYS:SG	1:B:480:ALA:HB1	2.52	0.50
1:F:270:ILE:O	1:F:270:ILE:HD12	2.11	0.50
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.77	0.50
1:G:222:LEU:HD11	1:G:301:ILE:N	2.27	0.50
1:G:385:THR:HG22	1:G:386:GLU:N	2.27	0.50
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.94	0.50
1:G:215:LEU:HB2	1:G:218:PRO:HG3	1.94	0.50
1:G:363:GLU:O	1:G:367:GLU:HG3	2.12	0.50
1:B:77:VAL:HG13	1:B:506:TYR:HB3	1.93	0.50
1:E:366:GLN:O	1:E:369:VAL:HG22	2.12	0.50
1:C:219:PHE:O	1:C:247:LEU:HD12	2.11	0.50
1:D:209:GLU:HG2	1:D:210:THR:N	2.26	0.50
1:C:313:THR:HG23	1:C:316:ASP:H	1.76	0.50
1:A:69:MET:CE	1:G:39:VAL:HG12	2.42	0.50
1:C:32:GLY:HA3	7:C:740:HOH:O	2.11	0.50
1:E:234:LEU:N	1:E:235:PRO:HD2	2.27	0.50
1:F:359:ASP:O	1:F:363:GLU:HG3	2.12	0.50
1:D:224:ASP:O	1:D:252:GLU:HB2	2.12	0.50
1:F:225:LYS:CG	1:F:303:GLU:HG3	2.34	0.50
1:F:363:GLU:O	1:F:367:GLU:HG3	2.11	0.50
1:D:385:THR:CG2	1:D:387:VAL:HG12	2.42	0.50
1:E:345:ARG:O	1:E:349:ILE:HG13	2.12	0.50
5:C:604:MPD:HM1	5:C:604:MPD:H52	1.94	0.50
1:D:180:GLY:HA3	1:D:380:LYS:HB3	1.93	0.50
1:C:229:ASN:OD1	1:C:259:LEU:HG	2.12	0.49
1:G:284:ARG:NH1	1:G:284:ARG:CG	2.71	0.49
1:G:366:GLN:HA	1:G:369:VAL:HG22	1.94	0.49
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.12	0.49
1:G:458:CYS:HB3	7:G:719:HOH:O	2.11	0.49
1:C:173:GLY:O	1:C:404:ARG:NH2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:PRO:HG3	1:F:310:GLU:CB	2.42	0.49
1:G:257:GLU:OE2	1:G:261:THR:HB	2.12	0.49
1:C:30:THR:HB	1:C:51:LYS:O	2.12	0.49
1:G:281:PHE:CB	1:G:282:GLY:HA2	2.41	0.49
1:B:231:ARG:HA	1:B:234:LEU:HG	1.93	0.49
1:F:164:GLU:HA	1:F:167[B]:ASP:OD2	2.12	0.49
1:F:153:ASN:OD1	7:F:706:HOH:O	2.20	0.49
1:B:259:LEU:HD12	1:B:260:ALA:H	1.76	0.49
1:G:385:THR:HG22	1:G:387:VAL:H	1.77	0.49
1:C:217:SER:N	1:C:321:LYS:O	2.39	0.49
1:F:183:LEU:CD1	1:F:184:GLN:H	2.25	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.94	0.49
1:C:288:MET:HA	1:C:291:ASP:HB2	1.93	0.49
1:D:198:GLY:HA3	1:D:327:LYS:O	2.13	0.49
1:G:178:GLU:O	1:G:381:VAL:HG23	2.11	0.49
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.94	0.49
1:D:224:ASP:OD1	1:D:286:LYS:HD3	2.12	0.49
1:D:25:ASP:OD1	1:D:28:LYS:HE2	2.13	0.49
1:F:203:TYR:HD2	1:F:263:VAL:HG13	1.76	0.49
1:E:261:THR:O	1:E:264:VAL:HB	2.12	0.49
1:E:383:ALA:O	1:E:384:ALA:HB3	2.13	0.49
1:D:128:VAL:CG1	1:D:132:LYS:HE3	2.43	0.49
1:B:392:LYS:HA	1:B:395:ARG:HE	1.77	0.49
1:F:203:TYR:HD2	1:F:263:VAL:CG1	2.24	0.49
1:A:383:ALA:CB	1:A:384:ALA:CA	2.69	0.49
1:C:225:LYS:O	1:C:227:ILE:HG13	2.13	0.49
1:C:200:LEU:HD12	1:C:254:VAL:HG23	1.94	0.49
1:D:152:ALA:CB	1:D:155:ASP:H	2.25	0.49
1:C:305:ILE:HG23	1:C:307:MET:HG3	1.95	0.49
1:G:248:LEU:HD21	1:G:250:ILE:CG2	2.42	0.49
1:G:301:ILE:CG2	1:G:307:MET:HG3	2.43	0.49
1:D:179:ASP:HB3	1:D:389:MET:HE2	1.94	0.49
1:D:385:THR:HG23	1:D:387:VAL:HG12	1.93	0.49
1:B:157:THR:HB	7:B:806:HOH:O	2.13	0.49
1:G:171:LYS:HB3	1:G:407:VAL:HG11	1.95	0.49
1:F:186:GLU:HG3	1:F:187:LEU:N	2.27	0.49
1:E:217:SER:HA	1:E:320:ALA:O	2.12	0.49
1:G:279:PRO:HB2	1:G:285:ARG:HA	1.94	0.49
1:D:200:LEU:CD1	1:D:254:VAL:HB	2.42	0.49
1:F:221:LEU:CD2	1:F:249:ILE:HD12	2.42	0.49
1:C:202:PRO:O	1:C:203:TYR:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ASN:C	1:D:271:VAL:HG12	2.32	0.49
1:C:279:PRO:HG2	1:C:288:MET:HE2	1.95	0.49
1:G:10:ASN:HB3	7:G:736:HOH:O	2.12	0.49
1:D:118[A]:ARG:NH2	7:D:785:HOH:O	2.46	0.49
1:G:24:ALA:O	1:G:28:LYS:HG2	2.12	0.49
1:E:258:ALA:O	1:E:262:LEU:HD13	2.13	0.49
1:G:197:ALA:CA	1:G:277:LYS:HG2	2.43	0.49
1:C:349:ILE:HG22	1:C:365:LEU:CD2	2.43	0.49
1:B:39:VAL:HG12	1:C:69:MET:HE1	1.95	0.49
1:B:181:THR:CG2	1:B:182:GLY:H	2.24	0.49
1:E:321:LYS:O	1:E:321:LYS:HD3	2.13	0.49
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.95	0.49
1:C:225:LYS:HZ3	1:C:259:LEU:HD22	1.78	0.48
1:C:243:ALA:HB3	1:C:244:GLY:C	2.32	0.48
1:B:225:LYS:HD2	1:B:303:GLU:OE2	2.13	0.48
1:E:215:LEU:HB2	1:E:323:VAL:HG22	1.94	0.48
1:G:493:ILE:HD13	2:G:601:ADP:C6	2.48	0.48
1:F:259:LEU:O	1:F:263:VAL:HG23	2.13	0.48
1:G:420:ILE:HD13	1:G:448:GLU:HG2	1.94	0.48
1:C:215:LEU:C	1:C:215:LEU:HD12	2.33	0.48
1:B:198:GLY:N	1:B:277:LYS:HE3	2.28	0.48
1:A:358:SER:HB3	1:A:361:ASP:OD2	2.13	0.48
1:C:458:CYS:SG	1:C:480:ALA:HB1	2.53	0.48
1:F:219:PHE:CE2	1:F:245:LYS:HD2	2.48	0.48
1:G:16:MET:HE2	1:G:73:MET:SD	2.54	0.48
1:D:385:THR:HG22	1:D:388:GLU:OE2	2.12	0.48
1:D:420:ILE:HD13	1:D:448:GLU:HG2	1.95	0.48
1:D:33:PRO:HG2	1:D:480:ALA:HB3	1.94	0.48
1:G:248:LEU:C	1:G:248:LEU:HD23	2.34	0.48
1:C:225:LYS:HE2	1:C:254:VAL:HA	1.95	0.48
1:A:69:MET:HE2	1:G:39:VAL:HG12	1.95	0.48
1:A:385:THR:HG22	1:A:386:GLU:N	2.28	0.48
1:E:403:THR:O	1:E:407:VAL:HG23	2.13	0.48
1:G:248:LEU:HD23	1:G:249:ILE:N	2.28	0.48
1:G:279:PRO:CG	1:G:285:ARG:HB2	2.44	0.48
1:F:201:SER:HB2	1:F:204:PHE:HE2	1.77	0.48
1:C:326:ASN:OD1	1:C:327:LYS:HG2	2.13	0.48
1:B:217:SER:HB3	1:B:245:LYS:HZ1	1.78	0.48
1:G:124:VAL:O	1:G:128:VAL:HG23	2.13	0.48
1:E:140:ASP:N	1:E:140:ASP:OD1	2.46	0.48
1:C:293:ALA:HB1	1:C:298:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ASN:HB2	1:C:270:ILE:HD11	1.95	0.48
1:C:325:ILE:CG1	1:C:326:ASN:N	2.76	0.48
1:B:381:VAL:CG1	1:B:392:LYS:HD3	2.43	0.48
1:F:171:LYS:O	1:F:404:ARG:NH1	2.44	0.48
1:F:186:GLU:CG	1:F:187:LEU:N	2.77	0.48
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.49	0.48
1:A:162:ILE:HG22	1:A:166:MET:HE2	1.95	0.48
1:C:199:TYR:HE1	1:C:202:PRO:CA	2.26	0.48
1:F:281:PHE:N	1:F:285:ARG:HB2	2.29	0.48
1:E:386:GLU:O	1:E:390:LYS:HG2	2.14	0.48
1:C:243:ALA:HB3	1:C:244:GLY:HA2	1.96	0.48
1:B:232:GLU:HA	1:B:310:GLU:CG	2.44	0.48
1:G:216:GLU:OE2	1:G:321:LYS:NZ	2.47	0.48
1:C:206:ASN:OD1	1:C:214:GLU:N	2.47	0.48
1:D:288:MET:O	1:D:291:ASP:HB2	2.13	0.48
1:C:172:GLU:OE1	1:C:172:GLU:N	2.40	0.48
1:G:222:LEU:CD2	1:G:300:VAL:HA	2.44	0.48
1:G:385:THR:CG2	1:G:387:VAL:HG12	2.43	0.48
1:C:35:GLY:O	1:C:51:LYS:HE2	2.14	0.48
1:G:242:LYS:O	1:G:243:ALA:HB3	2.14	0.48
1:B:263:VAL:O	1:B:267:MET:HG3	2.14	0.47
1:E:383:ALA:HB2	1:E:389:MET:HA	1.95	0.47
1:E:218:PRO:CB	1:E:246:PRO:HG2	2.32	0.47
1:F:313:THR:HG22	1:F:314:LEU:N	2.29	0.47
1:C:203:TYR:HB3	1:C:267:MET:SD	2.55	0.47
1:C:206:ASN:ND2	1:C:214:GLU:H	2.12	0.47
1:E:16:MET:HG2	1:E:514:MET:CE	2.44	0.47
1:G:219:PHE:C	1:G:220:ILE:HD12	2.35	0.47
1:G:223:ALA:HB1	1:G:225:LYS:N	2.28	0.47
1:G:383:ALA:HB1	1:G:388:GLU:CG	2.43	0.47
1:F:217:SER:N	1:F:321:LYS:O	2.35	0.47
1:G:383:ALA:HB2	1:G:392:LYS:CD	2.40	0.47
1:G:455:VAL:O	1:G:458:CYS:HB2	2.15	0.47
1:B:150:ILE:HD11	1:B:493:ILE:HA	1.97	0.47
1:A:261:THR:HG23	1:A:265:ASN:ND2	2.29	0.47
1:G:281:PHE:HB3	1:G:285:ARG:HD3	1.96	0.47
1:A:144:ILE:CG2	1:A:166:MET:HE3	2.43	0.47
1:F:225:LYS:NZ	1:F:308:GLU:HA	2.29	0.47
1:G:257:GLU:HG2	1:G:261:THR:OG1	2.15	0.47
1:F:204:PHE:HB3	1:F:266:THR:OG1	2.13	0.47
1:A:381:VAL:HG13	1:A:392:LYS:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:345:ARG:O	1:F:349:ILE:HG13	2.14	0.47
1:B:34:LYS:HE2	1:C:118[A]:ARG:HH22	1.79	0.47
1:E:264:VAL:O	1:E:268:ARG:HG3	2.13	0.47
1:A:229:ASN:HB3	1:A:232:GLU:OE1	2.14	0.47
1:B:38:VAL:HG22	1:C:519:CYS:HB3	1.97	0.47
1:C:227:ILE:HG22	1:C:228:SER:N	2.22	0.47
1:A:242:LYS:HE2	1:B:229:ASN:HB2	1.96	0.47
1:E:180:GLY:HA3	1:E:381:VAL:C	2.35	0.47
1:C:68:ASN:O	1:C:72:GLN:HG2	2.15	0.47
1:C:270:ILE:HG13	1:C:271:VAL:H	1.80	0.47
1:F:227:ILE:CD1	1:F:309:LEU:HD21	2.44	0.47
1:D:219:PHE:O	1:D:247:LEU:HD12	2.14	0.47
1:E:444:LEU:HD23	1:E:447:MET:HE1	1.96	0.47
1:C:349:ILE:HG22	1:C:365:LEU:HD23	1.96	0.47
1:A:284:ARG:O	1:A:288:MET:HG3	2.15	0.47
1:D:385:THR:HG23	1:D:388:GLU:HG2	1.97	0.47
1:C:489:ILE:HD13	1:C:494:LEU:CD2	2.44	0.47
1:B:149:THR:OG1	1:B:156:GLU:HA	2.14	0.47
1:A:253:ASP:HB3	7:A:725:HOH:O	2.14	0.47
1:E:417:VAL:HG21	1:E:488:MET:HG3	1.96	0.47
1:B:288:MET:O	1:B:292:ILE:HG13	2.14	0.47
1:G:15:LYS:HD3	1:G:66:PHE:HB2	1.97	0.47
1:G:325:ILE:N	1:G:325:ILE:HD12	2.30	0.47
1:G:219:PHE:CB	1:G:317:LEU:HD23	2.39	0.47
1:A:266:THR:HG22	1:A:270:ILE:HG21	1.96	0.47
1:G:222:LEU:HD11	1:G:300:VAL:CA	2.37	0.47
1:F:204:PHE:HB3	1:F:266:THR:HB	1.93	0.47
1:B:276:VAL:HG11	1:B:325:ILE:HD13	1.97	0.47
1:A:108:ALA:HB2	5:A:605:MPD:HM2	1.95	0.47
1:B:475:ASN:O	1:B:488:MET:HG2	2.14	0.47
1:E:420:ILE:HD13	1:E:448:GLU:HG2	1.96	0.47
1:C:243:ALA:N	1:C:244:GLY:HA2	2.29	0.47
1:F:383:ALA:CB	1:F:388:GLU:HB3	2.44	0.47
1:C:206:ASN:HD21	1:C:214:GLU:H	1.62	0.47
1:A:68:ASN:O	1:A:72:GLN:HG2	2.15	0.47
1:A:498:LYS:NZ	5:A:609:MPD:C5	2.78	0.47
1:C:336:VAL:O	1:C:336:VAL:HG12	2.15	0.47
1:G:392:LYS:O	1:G:396:VAL:HG23	2.14	0.46
1:A:176:THR:OG1	1:A:177:VAL:N	2.49	0.46
1:B:222:LEU:HD13	1:B:293:ALA:HB2	1.97	0.46
1:F:224:ASP:O	1:F:252:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLU:O	1:D:261:THR:OG1	2.23	0.46
1:G:14:VAL:O	1:G:18[B]:ARG:HG3	2.14	0.46
1:G:359:ASP:HA	1:G:362:ARG:NH2	2.30	0.46
5:B:605:MPD:O4	5:B:605:MPD:HM2	2.15	0.46
1:A:381:VAL:CG1	1:A:392:LYS:HD3	2.45	0.46
1:A:349:ILE:HB	1:A:369:VAL:HG12	1.96	0.46
1:D:445:ARG:NH2	7:D:730:HOH:O	2.48	0.46
1:G:221:LEU:HD12	1:G:249:ILE:CG1	2.45	0.46
1:G:251:ALA:HB2	1:G:279:PRO:CD	2.45	0.46
1:C:266:THR:OG1	1:C:272:LYS:HA	2.14	0.46
1:C:16:MET:HE2	1:C:73:MET:HE2	1.96	0.46
1:F:179:ASP:OD1	1:F:393:LYS:HD2	2.15	0.46
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.15	0.46
1:F:215:LEU:HB3	1:F:218:PRO:HB3	1.97	0.46
1:D:160:LYS:O	1:D:163:ALA:N	2.46	0.46
1:D:164:GLU:N	1:D:164:GLU:OE1	2.44	0.46
1:E:381:VAL:O	1:E:381:VAL:HG22	2.16	0.46
1:E:460:GLU:OE2	7:E:754:HOH:O	2.21	0.46
1:G:433:ASN:ND2	7:G:785:HOH:O	2.40	0.46
1:B:487:ASN:O	1:B:491:MET:HG3	2.16	0.46
1:D:360:TYR:O	1:D:364:LYS:HG2	2.16	0.46
1:B:204:PHE:HE1	1:B:263:VAL:HA	1.81	0.46
1:C:200:LEU:CD1	1:C:254:VAL:CG2	2.94	0.46
1:F:222:LEU:O	1:F:301:ILE:HG22	2.15	0.46
1:B:227:ILE:CD1	1:B:309:LEU:HD22	2.46	0.46
1:G:205:ILE:HA	1:G:213:VAL:CG2	2.45	0.46
1:C:261:THR:HA	1:C:264:VAL:CG1	2.45	0.46
1:F:165:ALA:O	1:F:169:VAL:HG22	2.16	0.46
1:D:166:MET:O	1:D:170:GLY:N	2.49	0.46
1:E:49:ILE:HD12	1:F:513:LEU:HD13	1.98	0.46
1:G:105:LYS:HG2	5:G:604:MPD:O4	2.14	0.46
1:C:231:ARG:NH1	1:C:258:ALA:HB1	2.31	0.46
1:B:227:ILE:HD12	1:B:309:LEU:CD2	2.46	0.46
1:C:348:GLN:O	1:C:352:GLN:HG3	2.15	0.46
1:A:498:LYS:NZ	5:A:609:MPD:H53	2.31	0.46
1:C:385:THR:HG22	1:C:386:GLU:H	1.81	0.46
1:F:381:VAL:CG2	1:F:392:LYS:HD3	2.45	0.46
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.56	0.46
1:E:219:PHE:CE2	1:E:245:LYS:HD3	2.51	0.46
1:A:270:ILE:CG2	1:A:271:VAL:C	2.84	0.46
1:E:444:LEU:CA	1:E:447:MET:HE3	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:VAL:HG22	1:G:265:ASN:N	2.30	0.46
1:F:264:VAL:O	1:F:268:ARG:HB2	2.16	0.46
1:D:166:MET:HG2	1:D:175:ILE:HD11	1.98	0.46
1:E:308:GLU:HB2	1:E:311:LYS:HD3	1.98	0.46
1:E:351:GLN:O	1:E:355:GLU:HG3	2.15	0.46
1:G:221:LEU:O	1:G:250:ILE:HG12	2.16	0.46
1:C:227:ILE:CG2	1:C:233:MET:HE3	2.46	0.46
1:G:268:ARG:HH22	1:G:271:VAL:CG2	2.29	0.46
1:A:381:VAL:CG1	1:A:392:LYS:HB3	2.45	0.46
1:B:305:ILE:CG2	1:B:307:MET:HG3	2.42	0.46
1:A:169:VAL:HG23	1:A:377:ALA:HB2	1.97	0.46
1:G:34:LYS:HG3	1:G:458:CYS:SG	2.56	0.46
1:C:230:ILE:HD12	1:C:262:LEU:HD12	1.98	0.45
1:G:321:LYS:HG3	1:G:322:ARG:N	2.30	0.45
1:G:247:LEU:HD12	1:G:248:LEU:H	1.81	0.45
1:D:253:ASP:OD1	1:D:254:VAL:N	2.49	0.45
1:B:363:GLU:O	1:B:367:GLU:HG3	2.15	0.45
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.98	0.45
1:C:265:ASN:ND2	1:C:270:ILE:HD11	2.31	0.45
1:G:301:ILE:HG23	1:G:307:MET:CG	2.44	0.45
1:C:243:ALA:HB3	1:C:245:LYS:N	2.31	0.45
1:A:224:ASP:OD1	1:A:286:LYS:HD2	2.17	0.45
1:F:14:VAL:O	1:F:18[B]:ARG:HG3	2.16	0.45
1:G:321:LYS:HZ2	1:G:322:ARG:HB2	1.81	0.45
1:G:281:PHE:CB	1:G:282:GLY:CA	2.86	0.45
1:F:242:LYS:O	1:G:257:GLU:HB2	2.17	0.45
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.98	0.45
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.99	0.45
1:B:123:ALA:HB2	1:B:440:ILE:HG23	1.97	0.45
1:D:226:LYS:HD2	1:D:255:GLU:CD	2.37	0.45
1:G:385:THR:HB	1:G:388:GLU:CB	2.41	0.45
1:D:385:THR:HG22	1:D:388:GLU:HG2	1.96	0.45
1:A:38:VAL:HG22	1:B:519:CYS:HB3	1.99	0.45
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.99	0.45
1:C:353:ILE:CD1	1:C:365:LEU:HD22	2.46	0.45
1:G:261:THR:C	1:G:264:VAL:HG13	2.36	0.45
1:G:220:ILE:N	1:G:220:ILE:HD12	2.32	0.45
1:B:215:LEU:HB3	1:B:218:PRO:HB3	1.99	0.45
1:E:102:GLU:HB2	1:E:442:VAL:HG13	1.98	0.45
1:E:193:MET:HE1	1:E:372:LEU:HD12	1.99	0.45
1:C:308:GLU:O	1:C:311:LYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:GLY:HA3	1:E:67:GLU:O	2.17	0.45
1:C:231:ARG:HH12	1:C:258:ALA:HB1	1.82	0.45
1:G:350:ARG:O	1:G:353:ILE:HG12	2.17	0.45
1:A:366:GLN:O	1:A:369:VAL:HG22	2.16	0.45
1:G:192:GLY:HA2	1:G:295:LEU:HD21	1.99	0.45
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.41	0.45
1:B:248:LEU:HD13	1:B:325:ILE:HD11	1.99	0.45
1:G:100:ILE:HD13	1:G:514:MET:SD	2.56	0.45
1:G:215:LEU:HB2	1:G:218:PRO:HG2	1.97	0.45
1:C:257:GLU:O	1:C:261:THR:HG23	2.17	0.45
1:F:381:VAL:HG22	1:F:392:LYS:HD3	1.97	0.45
1:G:155:ASP:HB3	1:G:158:VAL:CG1	2.46	0.45
1:G:262:LEU:O	1:G:262:LEU:HD12	2.17	0.45
1:G:277:LYS:O	1:G:278:ALA:HB3	2.16	0.45
1:C:200:LEU:CD1	1:C:254:VAL:HB	2.47	0.45
1:B:227:ILE:HG21	1:B:233:MET:CE	2.38	0.45
1:D:270:ILE:O	1:D:270:ILE:HG12	2.17	0.45
1:D:392:LYS:O	1:D:395:ARG:HB3	2.16	0.45
1:G:104:LEU:HB3	5:G:604:MPD:H12	1.99	0.45
1:F:25:ASP:OD1	1:F:28:LYS:HE2	2.16	0.45
1:G:68:ASN:O	1:G:72:GLN:HG2	2.17	0.45
1:B:188:ASP:N	1:B:188:ASP:OD1	2.49	0.45
1:D:273:VAL:HG22	1:D:274:ALA:N	2.32	0.45
1:A:230:ILE:O	1:A:230:ILE:HG12	2.16	0.44
1:C:259:LEU:HA	1:C:262:LEU:CD1	2.44	0.44
1:F:225:LYS:HZ2	1:F:309:LEU:HD12	1.82	0.44
1:C:179:ASP:HB3	1:C:389:MET:HE3	1.98	0.44
1:F:177:VAL:HG13	1:F:397:GLU:HG2	1.98	0.44
1:B:140:ASP:OD2	1:B:142:LYS:HB3	2.16	0.44
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.99	0.44
1:F:235:PRO:HG3	1:F:310:GLU:CA	2.48	0.44
1:A:401:HIS:O	1:A:404:ARG:HB2	2.16	0.44
1:C:213:VAL:CG1	1:C:325:ILE:HG23	2.47	0.44
1:C:198:GLY:HA3	1:C:327:LYS:O	2.17	0.44
1:A:344:GLY:O	1:A:348:GLN:HG3	2.17	0.44
1:B:455:VAL:HG21	1:B:465:VAL:HG11	1.98	0.44
1:G:285:ARG:HG3	1:G:289:LEU:HD12	2.00	0.44
1:C:259:LEU:C	1:C:262:LEU:HD13	2.38	0.44
1:A:456:LEU:HG	5:A:608:MPD:H12	2.00	0.44
1:C:352:GLN:HA	1:C:355:GLU:CD	2.38	0.44
1:A:16:MET:HB3	1:A:16:MET:HE2	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:O	1:A:128:VAL:HG23	2.17	0.44
1:C:25:ASP:O	1:C:29:VAL:HG13	2.17	0.44
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.17	0.44
1:A:475:ASN:O	1:A:488:MET:HG2	2.17	0.44
1:F:309:LEU:N	1:F:309:LEU:HD12	2.32	0.44
1:G:268:ARG:HH22	1:G:271:VAL:HG23	1.82	0.44
1:B:181:THR:CG2	1:B:182:GLY:N	2.81	0.44
1:A:193:MET:HG2	1:A:194:GLN:N	2.31	0.44
1:A:231:ARG:HA	1:A:234:LEU:HD23	1.99	0.44
1:D:218:PRO:HD2	1:D:320:ALA:O	2.17	0.44
1:D:359:ASP:O	1:D:363:GLU:HG3	2.18	0.44
1:F:420:ILE:HD13	1:F:448:GLU:HG2	1.99	0.44
1:C:230:ILE:HG21	1:C:258:ALA:HB1	1.98	0.44
1:D:136:VAL:HG13	1:D:137:PRO:CD	2.47	0.44
1:C:456:LEU:HD13	1:C:462:PRO:HG2	1.99	0.44
1:B:260:ALA:HA	1:B:263:VAL:CG1	2.48	0.44
1:F:225:LYS:HZ2	1:F:308:GLU:HA	1.83	0.44
1:G:385:THR:HG21	1:G:387:VAL:HG12	2.00	0.44
1:C:219:PHE:CG	1:C:245:LYS:HD2	2.53	0.44
1:A:498:LYS:HZ1	5:A:609:MPD:H53	1.82	0.44
1:D:152:ALA:HB3	1:D:154:SER:N	2.33	0.44
1:F:391:GLU:HG2	1:F:392:LYS:N	2.33	0.44
5:D:605:MPD:H11	5:D:605:MPD:O4	2.17	0.44
1:G:225:LYS:HA	1:G:226:LYS:HA	1.50	0.44
1:F:214:GLU:O	1:F:215:LEU:HD23	2.18	0.44
1:G:214:GLU:HA	1:G:323:VAL:O	2.17	0.44
1:B:225:LYS:NZ	1:B:232:GLU:OE2	2.27	0.44
1:B:319:GLN:O	1:B:336:VAL:HG23	2.18	0.44
1:C:177:VAL:HG21	1:C:397:GLU:CG	2.47	0.44
1:E:219:PHE:HE2	1:E:245:LYS:HD3	1.83	0.44
1:D:325:ILE:N	1:D:325:ILE:HD12	2.32	0.44
1:F:349:ILE:O	1:F:353:ILE:HG12	2.18	0.44
1:F:186:GLU:CD	1:F:187:LEU:H	2.22	0.44
1:A:348:GLN:O	1:A:352:GLN:HG3	2.18	0.44
1:E:117:LYS:NZ	7:E:750:HOH:O	2.51	0.44
1:D:336:VAL:O	1:D:336:VAL:HG12	2.18	0.44
1:E:200:LEU:CD1	1:E:254:VAL:HB	2.47	0.44
5:A:608:MPD:HM1	1:B:518:GLU:HG3	2.00	0.44
1:D:389:MET:HG3	1:D:390:LYS:N	2.33	0.44
1:A:365:LEU:CD2	1:A:368:ARG:HH21	2.31	0.44
1:B:238:GLU:O	1:B:242:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:SER:HA	1:E:202:PRO:HD3	1.89	0.44
1:D:326:ASN:OD1	1:D:329:THR:N	2.46	0.44
1:G:226:LYS:CB	1:G:227:ILE:HA	2.31	0.43
1:G:233:MET:HA	1:G:233:MET:HE3	1.99	0.43
1:A:140:ASP:OD1	1:A:140:ASP:N	2.50	0.43
1:B:332:ILE:N	1:B:332:ILE:HD12	2.33	0.43
1:E:177:VAL:CG1	1:E:397:GLU:HG2	2.48	0.43
1:G:18[A]:ARG:HG2	1:G:67:GLU:CD	2.38	0.43
1:E:81:ALA:HB1	7:E:719:HOH:O	2.17	0.43
2:E:601:ADP:O2A	2:E:601:ADP:O1B	2.36	0.43
1:F:313:THR:HG22	1:F:314:LEU:H	1.84	0.43
1:F:153:ASN:O	1:F:154:SER:HB2	2.18	0.43
1:F:195:PHE:CE2	1:F:330:THR:HG21	2.53	0.43
1:B:361:ASP:O	1:B:365:LEU:HD13	2.18	0.43
1:B:260:ALA:HA	1:B:263:VAL:HG12	2.00	0.43
1:C:326:ASN:OD1	1:C:327:LYS:N	2.44	0.43
1:G:16:MET:HB3	1:G:514:MET:CE	2.49	0.43
1:D:25:ASP:HA	1:D:28:LYS:HE2	2.00	0.43
1:D:522:THR:OG1	1:D:523:ASP:N	2.52	0.43
1:B:205:ILE:HG22	1:B:207:LYS:H	1.83	0.43
1:G:392:LYS:HE3	1:G:395:ARG:HH21	1.84	0.43
1:E:219:PHE:HB3	1:E:317:LEU:HD23	2.00	0.43
1:D:363:GLU:O	1:D:367:GLU:HG3	2.19	0.43
1:C:301:ILE:HD11	1:C:312:ALA:CB	2.48	0.43
1:G:251:ALA:CB	1:G:289:LEU:HD21	2.47	0.43
1:F:215:LEU:HD12	1:F:323:VAL:HG21	2.00	0.43
1:C:220:ILE:HD12	1:C:296:THR:CG2	2.46	0.43
1:F:192:GLY:HA3	1:F:376:VAL:HG23	2.00	0.43
1:C:256:GLY:CA	1:C:259:LEU:HD12	2.45	0.43
1:C:230:ILE:CG1	1:C:262:LEU:HD11	2.41	0.43
1:F:246:PRO:CB	1:F:272:LYS:HE3	2.46	0.43
1:A:393:LYS:NZ	1:A:397:GLU:OE2	2.38	0.43
1:A:37:ASN:CB	1:B:517:THR:HG22	2.49	0.43
1:B:362:ARG:O	1:B:366:GLN:HB2	2.18	0.43
1:G:27:VAL:HG12	1:G:90:THR:HG23	2.00	0.43
1:D:302:SER:O	1:D:307:MET:HB2	2.19	0.43
1:D:385:THR:O	1:D:389:MET:HB3	2.18	0.43
1:B:359:ASP:O	1:B:363:GLU:HG3	2.18	0.43
1:C:172:GLU:H	1:C:172:GLU:CD	2.22	0.43
1:E:160:LYS:O	1:E:164:GLU:HG3	2.19	0.43
1:B:15:LYS:NZ	1:B:64:ASP:OD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:THR:CG2	1:D:378:VAL:HG22	2.49	0.43
1:C:200:LEU:HD12	1:C:254:VAL:HB	2.01	0.43
1:A:162:ILE:HG22	1:A:166:MET:HE1	2.00	0.43
1:F:230:ILE:O	1:F:234:LEU:HG	2.19	0.43
1:C:219:PHE:CD2	1:C:245:LYS:HD2	2.53	0.43
1:F:383:ALA:HB1	1:F:388:GLU:CB	2.46	0.43
1:G:291:ASP:OD2	1:G:368:ARG:NH1	2.52	0.43
1:C:385:THR:HB	1:C:388:GLU:HB3	2.01	0.43
1:C:19:GLY:HA3	1:C:67:GLU:O	2.19	0.43
1:A:350:ARG:O	1:A:353:ILE:HB	2.19	0.43
1:B:198:GLY:H	1:B:277:LYS:CE	2.32	0.43
1:C:385:THR:O	1:C:389:MET:HB2	2.19	0.43
1:F:252:GLU:O	1:F:253:ASP:HB2	2.18	0.43
1:F:46:ALA:HA	1:F:47:PRO:HD3	1.83	0.43
1:G:219:PHE:HE1	1:G:245:LYS:HD3	1.83	0.42
1:C:272:LYS:HD2	1:C:272:LYS:N	2.34	0.42
1:F:221:LEU:CB	1:F:249:ILE:HD12	2.47	0.42
1:F:160:LYS:O	1:F:164:GLU:HG3	2.18	0.42
1:D:177:VAL:HG12	1:D:393:LYS:HG3	2.00	0.42
1:C:434:GLU:HG2	7:C:763:HOH:O	2.19	0.42
1:C:233:MET:SD	1:C:233:MET:N	2.92	0.42
1:C:352:GLN:HA	1:C:355:GLU:CG	2.50	0.42
1:G:321:LYS:HB3	1:G:334:ASP:HB3	2.00	0.42
1:F:185:ASP:N	1:F:185:ASP:OD1	2.39	0.42
1:F:200:LEU:CD1	1:F:254:VAL:HB	2.48	0.42
1:F:192:GLY:C	1:F:376:VAL:HG23	2.39	0.42
1:F:192:GLY:CA	1:F:376:VAL:HG23	2.48	0.42
1:C:225:LYS:HZ3	1:C:259:LEU:CD2	2.32	0.42
1:F:232:GLU:OE1	1:F:309:LEU:HD13	2.19	0.42
1:G:264:VAL:HG22	1:G:265:ASN:ND2	2.34	0.42
1:B:222:LEU:HD22	1:B:289:LEU:HD22	2.00	0.42
1:D:152:ALA:HB1	1:D:155:ASP:HB3	2.00	0.42
1:F:417:VAL:O	1:F:421:ARG:HG2	2.19	0.42
1:A:169:VAL:CG2	1:A:377:ALA:HB2	2.48	0.42
1:A:363:GLU:O	1:A:367:GLU:HG3	2.19	0.42
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.19	0.42
1:E:339:GLU:O	1:E:343:GLN:HG2	2.20	0.42
1:A:106:ALA:O	1:A:111:MET:HG3	2.19	0.42
1:G:251:ALA:CB	1:G:279:PRO:HD2	2.50	0.42
1:C:227:ILE:CG2	1:C:228:SER:H	2.16	0.42
1:E:383:ALA:HB1	1:E:388:GLU:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:GLY:CA	1:D:380:LYS:HB3	2.49	0.42
1:E:260:ALA:O	1:E:264:VAL:HG23	2.19	0.42
1:B:269:GLY:O	1:B:270:ILE:HB	2.19	0.42
1:B:364:LYS:HA	1:B:364:LYS:HD2	1.84	0.42
1:B:268:ARG:HH11	1:B:268:ARG:CG	2.29	0.42
1:F:349:ILE:HG21	1:F:369:VAL:HG13	2.01	0.42
1:C:456:LEU:HD13	1:C:462:PRO:CG	2.50	0.42
1:D:222:LEU:HD23	1:D:250:ILE:HB	2.01	0.42
1:A:195:PHE:CE1	1:A:330:THR:HB	2.55	0.42
1:D:232:GLU:OE2	1:D:309:LEU:HD12	2.19	0.42
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.83	0.42
1:D:14:VAL:O	1:D:18[B]:ARG:HG3	2.19	0.42
1:A:272:LYS:HB2	1:A:272:LYS:HE2	1.92	0.42
1:G:183:LEU:HA	1:G:384:ALA:HB2	2.02	0.42
1:C:226:LYS:HD3	1:C:252:GLU:OE2	2.19	0.42
1:D:266:THR:HA	1:D:271:VAL:HG13	2.02	0.42
1:C:207:LYS:O	1:C:207:LYS:HG3	2.20	0.42
1:D:143:ALA:O	1:D:147:VAL:HG23	2.20	0.42
1:G:279:PRO:HG2	1:G:285:ARG:HB2	2.01	0.42
1:C:266:THR:OG1	1:C:271:VAL:O	2.25	0.42
1:C:215:LEU:HD11	1:C:323:VAL:N	2.35	0.42
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.60	0.42
1:C:206:ASN:O	1:C:207:LYS:HG2	2.19	0.42
1:A:391:GLU:O	1:A:394:ALA:HB3	2.20	0.42
1:F:367:GLU:O	1:F:371:LYS:HG3	2.20	0.42
1:A:194:GLN:O	1:A:371:LYS:HE3	2.20	0.42
1:C:299:THR:HB	1:C:316:ASP:OD1	2.20	0.42
1:C:256:GLY:HA3	1:C:259:LEU:HB2	2.01	0.42
1:F:232:GLU:HG3	1:F:309:LEU:HD22	2.02	0.42
1:G:230:ILE:HA	1:G:233:MET:HG2	2.02	0.42
1:D:187:LEU:HD13	1:D:187:LEU:C	2.40	0.42
1:G:187:LEU:HD13	1:G:379:ILE:HG22	2.02	0.42
1:D:417:VAL:HG21	1:D:477:GLY:HA3	2.01	0.42
1:G:46:ALA:HA	1:G:47:PRO:HD3	1.84	0.42
1:C:27:VAL:HG12	1:C:90:THR:HG23	2.01	0.42
1:E:263:VAL:O	1:E:263:VAL:HG12	2.20	0.42
1:A:325:ILE:N	1:A:325:ILE:HD12	2.35	0.42
1:D:366:GLN:O	1:D:369:VAL:HG22	2.19	0.42
1:A:257:GLU:O	1:A:261:THR:HB	2.20	0.41
1:A:245:LYS:HE3	1:B:255:GLU:OE1	2.19	0.41
1:G:352:GLN:HA	1:G:355:GLU:CB	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:GLY:H	1:C:285:ARG:HH11	1.67	0.41
1:D:193:MET:HE3	1:D:371:LYS:HD3	2.02	0.41
1:F:501:ARG:HG2	1:F:505:GLN:OE1	2.20	0.41
1:F:350:ARG:HA	1:F:353:ILE:HG13	2.02	0.41
1:B:217:SER:HA	1:B:320:ALA:O	2.19	0.41
1:G:219:PHE:CE1	1:G:245:LYS:HD3	2.55	0.41
1:C:217:SER:O	1:C:245:LYS:HG3	2.20	0.41
1:F:183:LEU:N	1:F:183:LEU:HD12	2.35	0.41
1:C:209:GLU:HG2	1:C:210:THR:N	2.35	0.41
1:B:220:ILE:CD1	1:B:296:THR:HG21	2.50	0.41
1:E:184:GLN:HA	1:E:184:GLN:OE1	2.20	0.41
1:G:360:TYR:CE2	1:G:364:LYS:HE2	2.55	0.41
1:C:16:MET:SD	1:C:73:MET:HE1	2.60	0.41
1:E:102:GLU:OE1	1:E:445:ARG:NH1	2.53	0.41
1:F:253:ASP:OD1	1:F:277:LYS:HE2	2.20	0.41
1:D:16:MET:HG3	1:D:520:MET:SD	2.60	0.41
1:F:225:LYS:HE2	1:F:303:GLU:CG	2.51	0.41
1:G:321:LYS:HG3	1:G:322:ARG:HB2	2.02	0.41
1:E:49:ILE:CD1	1:F:513:LEU:HD13	2.50	0.41
1:D:207:LYS:HA	1:D:208:PRO:HD2	1.93	0.41
1:E:325:ILE:HD12	1:E:325:ILE:N	2.36	0.41
1:C:215:LEU:CD1	1:C:323:VAL:H	2.33	0.41
1:A:266:THR:CG2	1:A:270:ILE:HG21	2.50	0.41
1:F:364:LYS:HD3	1:F:367:GLU:OE1	2.21	0.41
1:C:393:LYS:NZ	1:C:397:GLU:OE2	2.53	0.41
1:A:461:GLU:HA	1:A:462:PRO:HD3	1.81	0.41
1:B:118[A]:ARG:HD2	7:B:786:HOH:O	2.20	0.41
1:D:39:VAL:HG12	1:E:69:MET:CE	2.51	0.41
7:E:745:HOH:O	1:F:518:GLU:HG2	2.18	0.41
1:C:215:LEU:HD11	1:C:218:PRO:HG3	2.02	0.41
1:A:270:ILE:CD1	1:A:273:VAL:HB	2.36	0.41
1:C:226:LYS:CE	1:C:226:LYS:HA	2.50	0.41
1:C:282:GLY:H	1:C:285:ARG:NH1	2.18	0.41
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.61	0.41
1:B:221:LEU:HD23	1:B:249:ILE:HG23	2.02	0.41
1:E:342:ILE:O	1:E:346:VAL:HG23	2.19	0.41
1:D:183:LEU:HD12	1:D:183:LEU:N	2.36	0.41
1:F:295:LEU:HD23	1:F:295:LEU:O	2.21	0.41
1:F:294:THR:HG23	1:F:341:ALA:HB1	2.02	0.41
1:B:259:LEU:HD12	1:B:260:ALA:CA	2.51	0.41
1:A:247:LEU:HB3	1:A:273:VAL:CG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:GLU:H	1:F:310:GLU:CD	2.21	0.41
1:A:514:MET:HE2	1:A:514:MET:HB3	1.66	0.41
1:D:227:ILE:HG22	1:D:258:ALA:CB	2.50	0.41
1:A:234:LEU:N	1:A:235:PRO:HD2	2.36	0.41
1:G:168:LYS:HD2	1:G:189:VAL:HG21	2.02	0.41
1:G:524:LEU:HA	1:G:524:LEU:HD23	1.88	0.41
1:C:256:GLY:O	1:C:260:ALA:N	2.53	0.41
1:A:177:VAL:HG11	1:A:397:GLU:CG	2.49	0.41
1:B:234:LEU:N	1:B:235:PRO:HD2	2.35	0.41
1:A:281:PHE:N	1:A:285:ARG:HB2	2.36	0.41
1:B:287:ALA:HB1	1:B:368:ARG:NH1	2.36	0.41
1:E:366:GLN:HG2	7:E:742:HOH:O	2.20	0.41
1:A:46:ALA:HA	1:A:47:PRO:HD3	1.93	0.41
1:G:284:ARG:NH1	1:G:364:LYS:HE3	2.35	0.41
1:C:350:ARG:O	1:C:353:ILE:HB	2.20	0.41
1:A:131:LEU:CD1	1:A:422:VAL:HG21	2.43	0.41
1:E:293:ALA:HB1	1:E:298:GLY:O	2.19	0.41
1:F:127:ALA:O	1:F:131:LEU:HB2	2.21	0.41
1:D:160:LYS:HG2	1:D:164:GLU:OE2	2.21	0.41
1:G:178:GLU:OE2	1:G:322:ARG:HD3	2.20	0.41
1:C:206:ASN:CG	1:C:214:GLU:H	2.24	0.41
1:D:68:ASN:O	1:D:72:GLN:HG2	2.21	0.41
1:G:223:ALA:CA	1:G:224:ASP:HB2	2.43	0.41
1:G:279:PRO:HB2	1:G:285:ARG:CA	2.51	0.41
1:F:193:MET:HB2	1:F:371:LYS:HB3	2.03	0.41
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.51	0.41
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.84	0.41
1:C:259:LEU:O	1:C:262:LEU:HD13	2.21	0.40
1:A:162:ILE:HD11	1:A:399:ALA:HB3	2.03	0.40
1:F:308:GLU:HB3	1:F:310:GLU:OE2	2.20	0.40
1:A:222:LEU:O	1:A:301:ILE:HG22	2.21	0.40
1:D:381:VAL:HG12	1:D:382:GLY:N	2.36	0.40
1:E:381:VAL:CG2	1:E:392:LYS:HD3	2.51	0.40
1:E:124:VAL:O	1:E:128:VAL:HG23	2.21	0.40
1:D:524:LEU:HA	1:D:525:PRO:HD3	1.97	0.40
1:D:455:VAL:HG21	1:D:465:VAL:HG11	2.03	0.40
1:F:234:LEU:N	1:F:235:PRO:CD	2.82	0.40
1:C:420:ILE:HD12	1:C:451:LEU:CD1	2.38	0.40
1:C:364:LYS:O	1:C:367:GLU:HB2	2.21	0.40
1:F:231:ARG:HG3	1:F:231:ARG:NH1	2.33	0.40
1:E:33:PRO:HG3	2:E:601:ADP:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HD2	1:A:303:GLU:OE1	2.21	0.40
1:F:326:ASN:HB3	1:F:329:THR:HB	2.02	0.40
1:A:30:THR:HB	1:A:51:LYS:O	2.21	0.40
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.21	0.40
1:E:163:ALA:O	1:E:167:ASP:HB2	2.22	0.40
1:C:273:VAL:HG22	1:C:274:ALA:N	2.35	0.40
5:D:604:MPD:O4	5:D:604:MPD:H12	2.21	0.40
1:D:193:MET:HB2	1:D:193:MET:HE2	1.92	0.40
1:C:39:VAL:HG12	1:D:69:MET:HE2	2.03	0.40
1:E:365:LEU:CD2	1:E:368:ARG:HH21	2.34	0.40
1:C:455:VAL:O	1:C:458:CYS:HB2	2.21	0.40
1:G:165:ALA:O	1:G:169:VAL:HG22	2.21	0.40
1:E:22:VAL:HG11	1:E:62:LEU:HD21	2.02	0.40
1:G:226:LYS:HB2	1:G:227:ILE:CA	2.44	0.40
1:D:181:THR:CB	1:E:277:LYS:HZ2	2.33	0.40
1:G:139:SER:HA	1:G:171:LYS:NZ	2.36	0.40
1:B:202:PRO:O	1:B:205:ILE:HG13	2.22	0.40
1:B:270:ILE:HG22	1:B:270:ILE:O	2.21	0.40
1:E:233:MET:HB3	1:E:233:MET:HE2	1.86	0.40
1:C:229:ASN:HA	1:C:259:LEU:CD1	2.51	0.40
1:F:77:VAL:HG21	1:F:510:VAL:HB	2.03	0.40
1:F:314:LEU:HA	1:F:317:LEU:HD12	2.03	0.40
1:B:16:MET:HG3	1:B:520:MET:CE	2.52	0.40
1:B:222:LEU:HD22	1:B:289:LEU:CD2	2.52	0.40
1:D:381:VAL:HG12	1:D:392:LYS:HD3	2.04	0.40
1:G:204:PHE:HB3	1:G:213:VAL:HG21	2.02	0.40
1:D:420:ILE:CD1	1:D:448:GLU:HG2	2.51	0.40
1:B:5:ASP:HB2	1:B:524:LEU:HD23	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:GLU:OE2	1:F:463:SER:OG[2_959]	2.11	0.09

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	523/548 (95%)	512 (98%)	11 (2%)	0	100	100
1	B	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	52	80
1	C	525/548 (96%)	505 (96%)	19 (4%)	1 (0%)	52	80
1	D	524/548 (96%)	509 (97%)	15 (3%)	0	100	100
1	E	523/548 (95%)	512 (98%)	10 (2%)	1 (0%)	52	80
1	F	526/548 (96%)	512 (97%)	13 (2%)	1 (0%)	52	80
1	G	523/548 (95%)	502 (96%)	21 (4%)	0	100	100
All	All	3667/3836 (96%)	3561 (97%)	102 (3%)	4 (0%)	56	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	ILE
1	F	270	ILE
1	E	270	ILE
1	C	227	ILE

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	403/413 (98%)	391 (97%)	12 (3%)	48	78
1	B	403/413 (98%)	395 (98%)	8 (2%)	63	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	405/413 (98%)	393 (97%)	12 (3%)	48 78
1	D	404/413 (98%)	392 (97%)	12 (3%)	48 78
1	E	403/413 (98%)	390 (97%)	13 (3%)	46 76
1	F	406/413 (98%)	397 (98%)	9 (2%)	60 86
1	G	403/413 (98%)	385 (96%)	18 (4%)	34 63
All	All	2827/2891 (98%)	2743 (97%)	84 (3%)	50 78

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	131	LEU
1	A	138	CYS
1	A	176	THR
1	A	177	VAL
1	A	226	LYS
1	A	261	THR
1	A	266	THR
1	A	301	ILE
1	A	305	ILE
1	A	328	ASP
1	A	329	THR
1	B	10	ASN
1	B	14	VAL
1	B	77	VAL
1	B	125	THR
1	B	136	VAL
1	B	213	VAL
1	B	268	ARG
1	B	277	LYS
1	C	77	VAL
1	C	136	VAL
1	C	213	VAL
1	C	226	LYS
1	C	263	VAL
1	C	264	VAL
1	C	268	ARG
1	C	276	VAL
1	C	319	GLN
1	C	325	ILE

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Mol	Chain	Res	Type
1	C	334	ASP
1	C	353	ILE
1	D	10	ASN
1	D	51	LYS
1	D	77	VAL
1	D	136	VAL
1	D	185	ASP
1	D	188	ASP
1	D	226	LYS
1	D	228	SER
1	D	261	THR
1	D	295	LEU
1	D	389	MET
1	D	401	HIS
1	E	16	MET
1	E	34	LYS
1	E	105	LYS
1	E	169	VAL
1	E	183	LEU
1	E	203	TYR
1	E	204	PHE
1	E	210	THR
1	E	268	ARG
1	E	273	VAL
1	E	359	ASP
1	E	381	VAL
1	E	393	LYS
1	F	10	ASN
1	F	77	VAL
1	F	177	VAL
1	F	183	LEU
1	F	264	VAL
1	F	268	ARG
1	F	270	ILE
1	F	353	ILE
1	F	473	ASP
1	G	11	ASP
1	G	18[A]	ARG
1	G	18[B]	ARG
1	G	77	VAL
1	G	140	ASP
1	G	141	SER

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Mol	Chain	Res	Type
1	G	150	ILE
1	G	158	VAL
1	G	176	THR
1	G	185	ASP
1	G	249	ILE
1	G	253	ASP
1	G	254	VAL
1	G	284	ARG
1	G	326	ASN
1	G	330	THR
1	G	350	ARG
1	G	401	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	10	ASN
1	E	146	GLN
1	F	401	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 27 are monoatomic - leaving 26 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	601	3,4	22,29,29	0.95	1 (4%)	27,45,45	2.21	7 (25%)
5	MPD	A	604	-	6,7,7	0.39	0	7,10,10	0.31	0
5	MPD	A	605	-	6,7,7	0.37	0	7,10,10	0.58	0
5	MPD	A	606	-	6,7,7	0.37	0	7,10,10	0.65	0
5	MPD	A	607	-	6,7,7	0.34	0	7,10,10	0.47	0
5	MPD	A	608	-	6,7,7	0.32	0	7,10,10	0.66	0
5	MPD	A	609	-	6,7,7	0.23	0	7,10,10	0.63	0
2	ADP	B	601	3,4	22,29,29	1.08	2 (9%)	27,45,45	2.08	6 (22%)
5	MPD	B	604	-	6,7,7	0.39	0	7,10,10	0.49	0
5	MPD	B	605	-	6,7,7	0.34	0	7,10,10	0.68	0
5	MPD	B	606	-	6,7,7	0.38	0	7,10,10	0.50	0
5	MPD	B	607	-	6,7,7	0.32	0	7,10,10	0.47	0
5	MPD	B	608	-	6,7,7	0.36	0	7,10,10	0.41	0
2	ADP	C	601	3,4	22,29,29	0.97	1 (4%)	27,45,45	2.12	6 (22%)
5	MPD	C	604	-	6,7,7	0.41	0	7,10,10	0.58	0
2	ADP	D	601	3,4	22,29,29	1.02	2 (9%)	27,45,45	2.35	7 (25%)
5	MPD	D	604	-	6,7,7	0.34	0	7,10,10	0.36	0
5	MPD	D	605	-	6,7,7	0.33	0	7,10,10	0.55	0
5	MPD	D	606	-	6,7,7	0.40	0	7,10,10	0.57	0
2	ADP	E	601	3,4	22,29,29	0.99	1 (4%)	27,45,45	2.16	6 (22%)
5	MPD	E	604	-	6,7,7	0.39	0	7,10,10	0.47	0
2	ADP	F	601	3,4	22,29,29	0.98	1 (4%)	27,45,45	2.06	4 (14%)
5	MPD	F	604	-	6,7,7	0.33	0	7,10,10	0.56	0
2	ADP	G	601	3,4	22,29,29	1.06	2 (9%)	27,45,45	2.06	7 (25%)
5	MPD	G	604	-	6,7,7	0.37	0	7,10,10	0.55	0
5	MPD	G	605	-	6,7,7	0.83	0	7,10,10	1.07	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	ADP	A	601	3,4	-	0/12/32/32	0/3/3/3
5	MPD	A	604	-	-	0/5/5/5	0/0/0/0
5	MPD	A	605	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	606	-	-	0/5/5/5	0/0/0/0
5	MPD	A	607	-	-	0/5/5/5	0/0/0/0
5	MPD	A	608	-	-	0/5/5/5	0/0/0/0
5	MPD	A	609	-	-	0/5/5/5	0/0/0/0
2	ADP	B	601	3,4	-	0/12/32/32	0/3/3/3
5	MPD	B	604	-	-	0/5/5/5	0/0/0/0
5	MPD	B	605	-	-	0/5/5/5	0/0/0/0
5	MPD	B	606	-	-	0/5/5/5	0/0/0/0
5	MPD	B	607	-	-	0/5/5/5	0/0/0/0
5	MPD	B	608	-	-	0/5/5/5	0/0/0/0
2	ADP	C	601	3,4	-	0/12/32/32	0/3/3/3
5	MPD	C	604	-	-	0/5/5/5	0/0/0/0
2	ADP	D	601	3,4	-	0/12/32/32	0/3/3/3
5	MPD	D	604	-	-	0/5/5/5	0/0/0/0
5	MPD	D	605	-	-	0/5/5/5	0/0/0/0
5	MPD	D	606	-	-	0/5/5/5	0/0/0/0
2	ADP	E	601	3,4	-	0/12/32/32	0/3/3/3
5	MPD	E	604	-	-	0/5/5/5	0/0/0/0
2	ADP	F	601	3,4	-	0/12/32/32	0/3/3/3
5	MPD	F	604	-	-	0/5/5/5	0/0/0/0
2	ADP	G	601	3,4	-	0/12/32/32	0/3/3/3
5	MPD	G	604	-	-	0/5/5/5	0/0/0/0
5	MPD	G	605	-	-	0/5/5/5	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	ADP	C2-N3	2.04	1.35	1.32
2	B	601	ADP	O4'-C1'	2.10	1.43	1.41
2	D	601	ADP	O4'-C1'	2.27	1.44	1.41
2	C	601	ADP	C5-C4	2.70	1.46	1.40
2	D	601	ADP	C5-C4	2.77	1.46	1.40
2	A	601	ADP	C5-C4	2.79	1.46	1.40
2	E	601	ADP	C5-C4	2.87	1.47	1.40
2	G	601	ADP	C5-C4	2.90	1.47	1.40
2	F	601	ADP	C5-C4	2.95	1.47	1.40
2	B	601	ADP	C5-C4	2.98	1.47	1.40

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ADP	N3-C2-N1	-7.89	122.85	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	ADP	N3-C2-N1	-7.72	122.98	128.89
2	F	601	ADP	N3-C2-N1	-7.52	123.13	128.89
2	C	601	ADP	N3-C2-N1	-7.29	123.31	128.89
2	D	601	ADP	N3-C2-N1	-7.25	123.34	128.89
2	B	601	ADP	N3-C2-N1	-6.58	123.86	128.89
2	G	601	ADP	N3-C2-N1	-5.67	124.55	128.89
2	B	601	ADP	PA-O3A-PB	-4.04	119.13	132.67
2	D	601	ADP	C2'-C1'-N9	-3.85	108.40	114.29
2	D	601	ADP	C1'-N9-C4	-3.76	121.27	126.94
2	E	601	ADP	PA-O3A-PB	-3.68	120.32	132.67
2	F	601	ADP	PA-O3A-PB	-3.60	120.59	132.67
2	G	601	ADP	PA-O3A-PB	-3.51	120.89	132.67
2	G	601	ADP	C2'-C1'-N9	-3.24	109.34	114.29
2	C	601	ADP	C2'-C1'-N9	-3.13	109.52	114.29
2	B	601	ADP	C4-C5-N7	-3.10	106.62	109.48
2	A	601	ADP	C2'-C1'-N9	-3.10	109.55	114.29
2	E	601	ADP	C4-C5-N7	-3.09	106.64	109.48
2	D	601	ADP	PA-O3A-PB	-3.08	122.35	132.67
2	D	601	ADP	C4-C5-N7	-3.00	106.72	109.48
2	E	601	ADP	C2'-C1'-N9	-2.98	109.74	114.29
2	F	601	ADP	C4-C5-N7	-2.89	106.82	109.48
2	B	601	ADP	C1'-N9-C4	-2.86	122.63	126.94
2	G	601	ADP	C4-C5-N7	-2.86	106.85	109.48
2	A	601	ADP	PA-O3A-PB	-2.80	123.27	132.67
2	C	601	ADP	C4-C5-N7	-2.76	106.94	109.48
2	A	601	ADP	C4-C5-N7	-2.74	106.96	109.48
2	C	601	ADP	C1'-N9-C4	-2.56	123.08	126.94
2	A	601	ADP	C1'-N9-C4	-2.39	123.34	126.94
2	D	601	ADP	O3A-PA-O5'	-2.27	96.91	102.94
2	A	601	ADP	C4'-O4'-C1'	-2.10	107.41	109.72
2	E	601	ADP	C1'-N9-C4	-2.08	123.80	126.94
2	C	601	ADP	C4'-O4'-C1'	-2.08	107.44	109.72
2	B	601	ADP	C2'-C1'-N9	-2.07	111.12	114.29
2	F	601	ADP	O3A-PA-O5'	-2.07	97.44	102.94
2	G	601	ADP	O3A-PA-O5'	-2.00	97.62	102.94
2	G	601	ADP	N6-C6-N1	2.55	124.69	119.20
2	E	601	ADP	O4'-C1'-N9	2.81	113.98	108.10
2	A	601	ADP	O4'-C1'-N9	2.82	114.00	108.10
2	B	601	ADP	O4'-C1'-N9	3.21	114.82	108.10
2	G	601	ADP	O4'-C1'-N9	3.71	115.86	108.10
2	C	601	ADP	O4'-C1'-N9	3.80	116.05	108.10
2	D	601	ADP	O4'-C1'-N9	4.42	117.34	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	MPD	1	0
5	A	605	MPD	2	0
5	A	606	MPD	3	0
5	A	608	MPD	3	0
5	A	609	MPD	4	0
5	B	604	MPD	2	0
5	B	605	MPD	1	0
5	B	608	MPD	2	0
5	C	604	MPD	1	0
5	D	604	MPD	1	0
5	D	605	MPD	1	0
2	E	601	ADP	2	0
5	E	604	MPD	2	0
2	G	601	ADP	1	0
5	G	604	MPD	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	524/548 (95%)	0.05	19 (3%) 46 47	27, 69, 168, 196	0
1	B	524/548 (95%)	0.05	22 (4%) 40 40	24, 60, 160, 190	0
1	C	524/548 (95%)	0.39	66 (12%) 5 4	26, 68, 202, 243	0
1	D	524/548 (95%)	-0.11	10 (1%) 70 71	30, 71, 155, 181	0
1	E	524/548 (95%)	-0.03	13 (2%) 61 61	31, 79, 141, 187	0
1	F	524/548 (95%)	0.09	35 (6%) 21 20	33, 75, 178, 223	0
1	G	524/548 (95%)	0.43	59 (11%) 7 5	30, 71, 211, 243	0
All	All	3668/3836 (95%)	0.12	224 (6%) 25 24	24, 72, 181, 243	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	225	LYS	9.9
1	G	251	ALA	8.8
1	G	233	MET	8.5
1	E	271	VAL	8.2
1	G	223	ALA	7.3
1	G	301	ILE	7.2
1	C	309	LEU	7.0
1	B	270	ILE	6.8
1	C	307	MET	6.4
1	G	203	TYR	6.4
1	G	286	LYS	6.1
1	G	181	THR	5.7
1	C	212	ALA	5.6
1	C	250	ILE	5.5
1	G	247	LEU	5.4
1	C	271	VAL	5.2
1	G	226	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	271	VAL	5.1
1	C	243	ALA	5.0
1	G	271	VAL	5.0
1	F	347	ALA	5.0
1	C	236	VAL	4.9
1	F	266	THR	4.8
1	C	249	ILE	4.8
1	C	305	ILE	4.7
1	C	203	TYR	4.7
1	G	266	THR	4.6
1	G	361	ASP	4.6
1	C	240	VAL	4.6
1	C	226	LYS	4.6
1	C	244	GLY	4.6
1	G	305	ILE	4.5
1	E	267	MET	4.5
1	C	306	GLY	4.4
1	G	314	LEU	4.4
1	G	224	ASP	4.3
1	F	201	SER	4.3
1	C	231	ARG	4.3
1	E	383	ALA	4.3
1	E	272	LYS	4.2
1	C	383	ALA	4.2
1	G	253	ASP	4.2
1	F	227	ILE	4.1
1	C	228	SER	4.1
1	F	240	VAL	4.0
1	B	356	ALA	4.0
1	G	252	GLU	3.9
1	G	302	SER	3.9
1	C	304	GLU	3.8
1	G	387	VAL	3.8
1	G	308	GLU	3.8
1	C	275	ALA	3.8
1	G	208	PRO	3.8
1	C	281	PHE	3.7
1	B	360	TYR	3.7
1	G	250	ILE	3.7
1	C	232	GLU	3.7
1	F	229	ASN	3.7
1	F	262	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	270	ILE	3.6
1	G	204	PHE	3.6
1	C	248	LEU	3.6
1	A	357	THR	3.6
1	A	222	LEU	3.6
1	B	268	ARG	3.6
1	G	306	GLY	3.6
1	C	344	GLY	3.5
1	B	208	PRO	3.4
1	B	272	LYS	3.4
1	G	356	ALA	3.4
1	F	270	ILE	3.4
1	A	268	ARG	3.4
1	C	200	LEU	3.4
1	G	227	ILE	3.4
1	G	304	GLU	3.4
1	G	273	VAL	3.4
1	F	44	PHE	3.3
1	G	317	LEU	3.3
1	G	281	PHE	3.3
1	C	280	GLY	3.3
1	G	277	LYS	3.3
1	F	233	MET	3.3
1	C	195	PHE	3.3
1	G	315	GLU	3.2
1	C	204	PHE	3.2
1	B	340	ALA	3.2
1	E	320	ALA	3.2
1	G	222	LEU	3.2
1	B	357	THR	3.2
1	C	257	GLU	3.2
1	G	358	SER	3.2
1	B	271	VAL	3.1
1	C	302	SER	3.1
1	C	279	PRO	3.1
1	A	266	THR	3.1
1	A	349	ILE	3.1
1	G	258	ALA	3.1
1	G	300	VAL	3.1
1	G	386	GLU	3.0
1	C	300	VAL	3.0
1	G	276	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	231	ARG	3.0
1	F	239	ALA	3.0
1	G	379	ILE	3.0
1	F	200	LEU	3.0
1	C	227	ILE	3.0
1	B	262	LEU	2.9
1	G	310	GLU	2.9
1	C	208	PRO	2.9
1	D	267	MET	2.9
1	F	259	LEU	2.9
1	C	270	ILE	2.9
1	C	363	GLU	2.9
1	C	253	ASP	2.9
1	D	212	ALA	2.9
1	F	260	ALA	2.9
1	B	269	GLY	2.9
1	G	249	ILE	2.9
1	F	300	VAL	2.9
1	B	244	GLY	2.8
1	G	267	MET	2.8
1	A	336	VAL	2.8
1	A	305	ILE	2.8
1	F	204	PHE	2.8
1	B	233	MET	2.8
1	C	233	MET	2.8
1	D	381	VAL	2.8
1	E	266	THR	2.8
1	C	215	LEU	2.8
1	A	264	VAL	2.8
1	D	203	TYR	2.8
1	A	267	MET	2.7
1	C	359	ASP	2.7
1	F	268	ARG	2.7
1	C	360	TYR	2.7
1	E	203	TYR	2.7
1	C	255	GLU	2.7
1	C	353	ILE	2.7
1	D	204	PHE	2.7
1	C	315	GLU	2.7
1	G	354	GLU	2.6
1	E	268	ARG	2.6
1	C	254	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	213	VAL	2.6
1	F	230	ILE	2.6
1	B	373	ALA	2.6
1	F	202	PRO	2.6
1	F	261	THR	2.6
1	D	44	PHE	2.6
1	F	203	TYR	2.6
1	F	267	MET	2.5
1	B	201	SER	2.5
1	C	201	SER	2.5
1	C	301	ILE	2.5
1	G	313	THR	2.5
1	F	231	ARG	2.5
1	C	361	ASP	2.5
1	F	251	ALA	2.5
1	C	237	LEU	2.5
1	A	44	PHE	2.5
1	D	387	VAL	2.5
1	G	213	VAL	2.5
1	C	263	VAL	2.4
1	A	351	GLN	2.4
1	C	269	GLY	2.4
1	D	269	GLY	2.4
1	B	263	VAL	2.4
1	C	362	ARG	2.4
1	D	305	ILE	2.4
1	G	215	LEU	2.4
1	E	270	ILE	2.4
1	C	303	GLU	2.4
1	F	212	ALA	2.4
1	G	303	GLU	2.3
1	A	362	ARG	2.3
1	B	254	VAL	2.3
1	C	223	ALA	2.3
1	C	220	ILE	2.3
1	C	284	ARG	2.3
1	C	274	ALA	2.3
1	C	318	GLY	2.3
1	C	199	TYR	2.3
1	B	238	GLU	2.3
1	F	247	LEU	2.3
1	A	172	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	301	ILE	2.3
1	G	275	ALA	2.3
1	A	353	ILE	2.3
1	C	358	SER	2.2
1	B	240	VAL	2.2
1	C	264	VAL	2.2
1	B	223	ALA	2.2
1	E	223	ALA	2.2
1	G	357	THR	2.2
1	F	265	ASN	2.2
1	E	209	GLU	2.2
1	C	268	ARG	2.2
1	F	234	LEU	2.2
1	E	265	ASN	2.2
1	C	320	ALA	2.2
1	A	272	LYS	2.1
1	F	228	SER	2.1
1	G	311	LYS	2.1
1	G	282	GLY	2.1
1	C	267	MET	2.1
1	C	295	LEU	2.1
1	F	264	VAL	2.1
1	A	231	ARG	2.1
1	C	230	ILE	2.1
1	B	204	PHE	2.1
1	F	311	LYS	2.1
1	G	232	GLU	2.1
1	E	264	VAL	2.1
1	G	240	VAL	2.1
1	D	268	ARG	2.1
1	G	283	ASP	2.1
1	G	362	ARG	2.1
1	F	269	GLY	2.1
1	A	304	GLU	2.1
1	C	283	ASP	2.0
1	B	301	ILE	2.0
1	F	305	ILE	2.0
1	G	307	MET	2.0
1	G	332	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
4	K	C	603	1/1	0.96	0.22	20.09	79,79,79,79	0
5	MPD	A	606	8/8	0.87	0.37	17.13	98,111,115,115	0
5	MPD	B	605	8/8	0.91	0.33	14.36	89,107,112,123	0
5	MPD	E	604	8/8	0.76	0.39	13.06	120,123,127,127	0
5	MPD	A	609	8/8	0.87	0.41	10.02	110,122,129,134	0
5	MPD	C	604	8/8	0.90	0.31	9.72	102,107,112,117	0
5	MPD	G	604	8/8	0.80	0.37	9.66	78,99,109,117	0
5	MPD	B	607	8/8	0.89	0.31	9.40	92,108,124,126	0
5	MPD	A	608	8/8	0.90	0.37	9.32	103,110,120,123	0
5	MPD	B	604	8/8	0.89	0.24	6.83	52,80,90,92	0
4	K	B	603	1/1	0.98	0.22	6.19	62,62,62,62	0
5	MPD	D	605	8/8	0.81	0.35	5.91	108,112,116,116	0
4	K	A	603	1/1	0.99	0.21	5.52	58,58,58,58	0
4	K	F	603	1/1	1.00	0.27	4.83	60,60,60,60	0
5	MPD	F	604	8/8	0.86	0.30	4.35	119,124,125,130	0
5	MPD	D	604	8/8	0.88	0.26	3.85	95,110,115,123	0
5	MPD	B	608	8/8	0.80	0.28	3.83	93,98,109,118	0
5	MPD	A	605	8/8	0.91	0.26	3.72	90,96,105,107	0
4	K	G	603	1/1	0.99	0.19	2.45	65,65,65,65	0
6	CA	D	607	1/1	0.97	0.18	2.24	118,118,118,118	0
2	ADP	B	601	27/27	0.98	0.19	2.15	30,48,62,127	0
6	CA	G	607	1/1	0.82	0.20	2.14	114,114,114,114	0
2	ADP	G	601	27/27	0.98	0.17	1.60	41,50,65,94	0
2	ADP	F	601	27/27	0.98	0.19	1.51	38,62,74,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	A	601	27/27	0.98	0.16	1.25	39,56,64,75	0
2	ADP	C	601	27/27	0.98	0.17	0.91	43,55,64,66	0
2	ADP	D	601	27/27	0.98	0.17	0.46	36,57,70,80	0
2	ADP	E	601	27/27	0.97	0.15	0.29	57,70,80,250	0
4	K	D	603	1/1	0.98	0.16	0.14	64,64,64,64	0
5	MPD	A	604	8/8	0.80	0.20	-0.16	106,109,115,123	0
6	CA	B	609	1/1	0.86	0.13	-0.33	141,141,141,141	0
3	MG	D	602	1/1	0.99	0.13	-	30,30,30,30	0
6	CA	E	607	1/1	0.78	0.20	-	126,126,126,126	0
6	CA	A	610	1/1	0.95	0.20	-	129,129,129,129	0
6	CA	E	606	1/1	0.93	0.07	-	111,111,111,111	0
6	CA	G	606	1/1	0.97	0.21	-	88,88,88,88	0
4	K	G	608	1/1	0.71	0.22	-	154,154,154,154	0
3	MG	F	602	1/1	0.97	0.11	-	28,28,28,28	0
5	MPD	D	606	8/8	0.86	0.28	-	79,99,108,113	0
4	K	E	603	1/1	0.96	0.14	-	89,89,89,89	0
5	MPD	G	605	8/8	0.84	0.32	-	114,117,141,153	0
6	CA	A	611	1/1	0.93	0.37	-	107,107,107,107	0
6	CA	E	605	1/1	0.92	0.12	-	108,108,108,108	0
3	MG	G	602	1/1	0.98	0.14	-	25,25,25,25	0
3	MG	B	602	1/1	0.91	0.18	-	29,29,29,29	0
3	MG	C	602	1/1	0.97	0.13	-	34,34,34,34	0
5	MPD	A	607	8/8	0.90	0.23	-	83,95,97,104	0
3	MG	A	602	1/1	0.94	0.15	-	33,33,33,33	0
5	MPD	B	606	8/8	0.88	0.23	-	74,90,103,111	0
6	CA	G	609	1/1	0.81	0.36	-	123,123,123,123	0
3	MG	E	602	1/1	0.98	0.11	-	38,38,38,38	0
4	K	F	605	1/1	0.40	0.48	-	166,166,166,166	0
6	CA	F	606	1/1	0.97	0.11	-	110,110,110,110	0

6.5 Other polymers (i)

There are no such residues in this entry.