



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:31 pm BST

PDB ID : 4KI8
Title : Crystal structure of a GroEL-ADP complex in the relaxed allosteric state
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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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

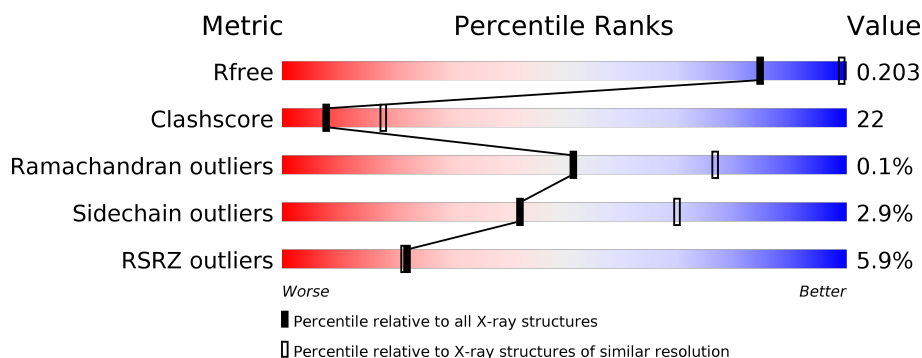
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	B	548	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>• •</div> </div> </div>
1	C	548	<div> <div>12%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>
1	D	548	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	E	548	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• •</div> </div> </div>
1	F	548	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	548	

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
4	K	F	605	-	-	-	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.

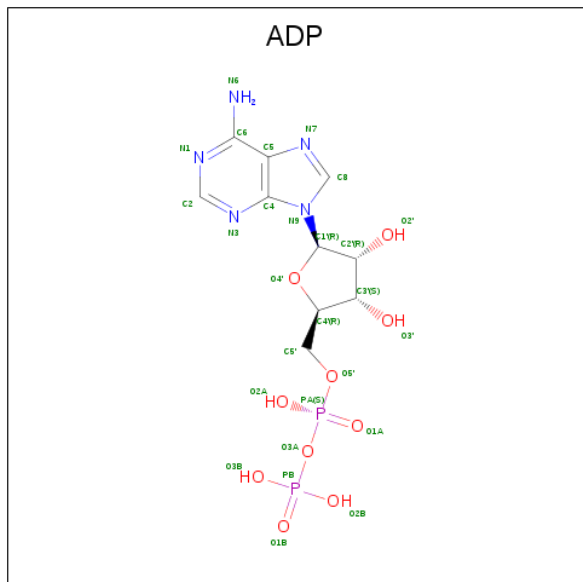
- Molecule 1 is a protein called GroEL protein.

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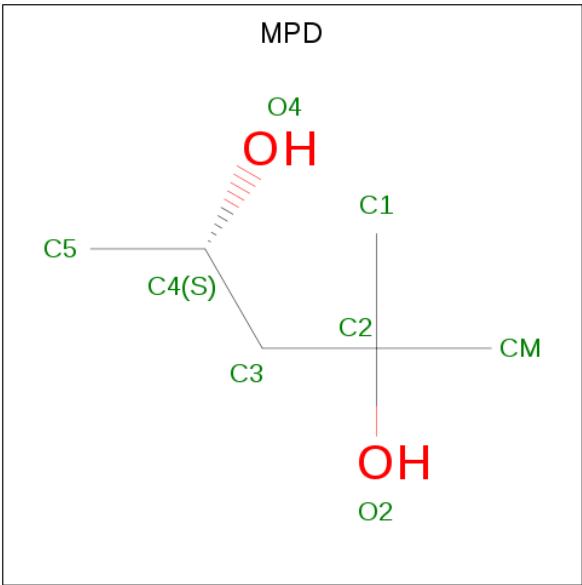
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

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

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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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	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	0	0
			8	6	2		
5	E	1	Total	C	O	0	0
			8	6	2		
5	F	1	Total	C	O	0	0
			8	6	2		
5	G	1	Total	C	O	0	0
			8	6	2		
5	G	1	Total	C	O	0	0
			8	6	2		

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

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

- Molecule 7 is water.

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

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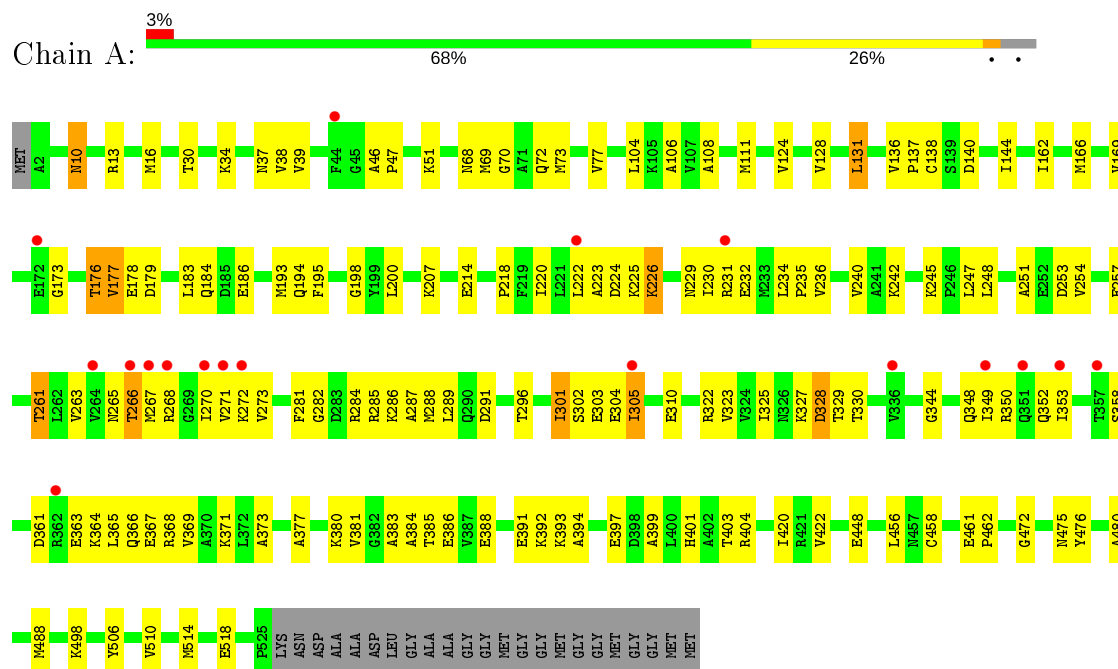
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	85	Total	O	0	0
			85	85		

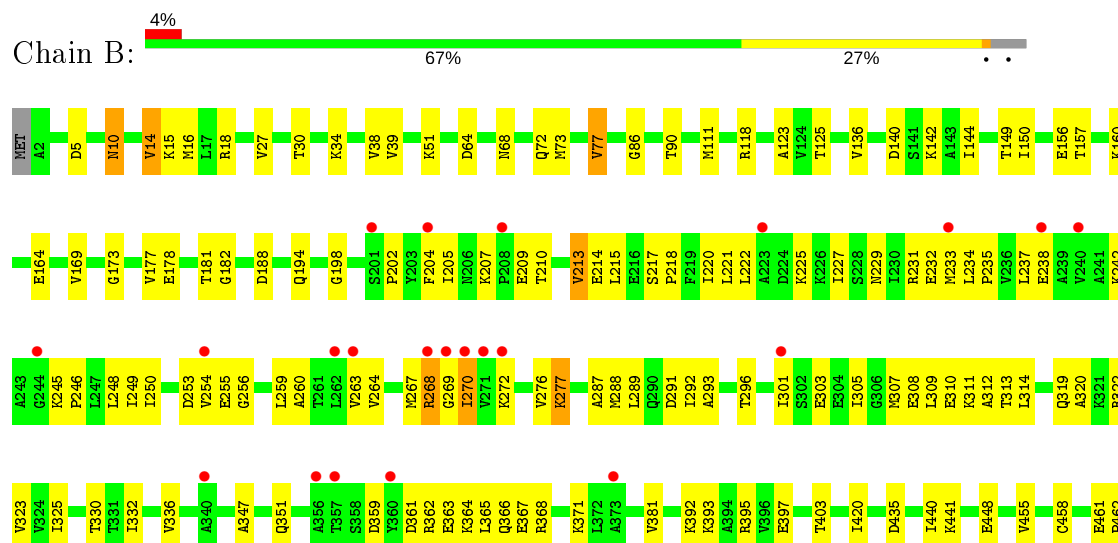
3 Residue-property plots

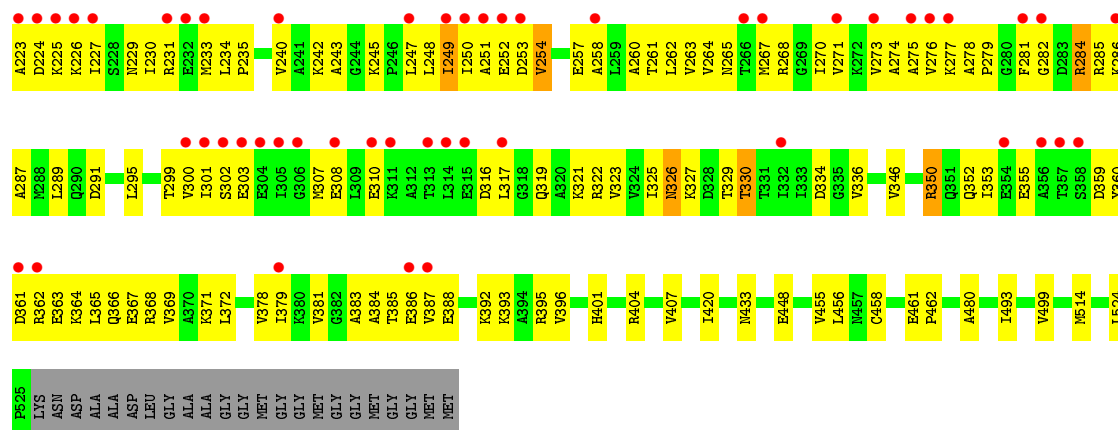
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: GroEL protein





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.166 , 0.203 0.167 , 0.203	Depositor DCC
R_{free} test set	2000 reflections (1.66%)	wwPDB-VP
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 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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: 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 [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	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:F:215:LEU:HB2	1:F:323:VAL:HG22	1.49	0.94
1:G:278:ALA:HB1	1:G:279:PRO:HD2	1.50	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:C:222:LEU:HB3	1:C:300:VAL:HG23	1.55	0.89
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.54	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
5:A:608:MPD:H52	5:A:608:MPD:H11	1.59	0.85
1:G:281:PHE:HB3	1:G:285:ARG:CB	2.06	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:B:39:VAL:HG21	1:C:16:MET:HE1	1.65	0.79
1:G:251:ALA:HB1	1:G:252:GLU:HB2	1.62	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:C:225:LYS:CB	1:C:251:ALA:HB1	2.12	0.77
1:G:221:LEU:HD11	1:G:247:LEU:HD21	1.65	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:F:301:ILE:CD1	1:F:307:MET:HB3	2.14	0.77
1:G:225:LYS:HB3	1:G:226:LYS:HG2	1.67	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:C:215:LEU:HD11	1:C:323:VAL:CB	2.16	0.76
1:E:183:LEU:CD1	1:E:384:ALA:HB2	2.14	0.76
1:G:281:PHE:CB	1:G:285:ARG:HB3	2.07	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:C:178:GLU:HG2	1:C:322:ARG:NH1	2.01	0.76
1:E:444:LEU:HD23	1:E:447:MET:HE3	1.68	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:B:305:ILE:HG23	1:B:307:MET:HG3	1.68	0.74
1:G:185:ASP:OD1	1:G:185:ASP:N	2.20	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:E:444:LEU:HD23	1:E:447:MET:CE	2.18	0.73
1:G:249:ILE:O	1:G:275:ALA:HA	1.88	0.73
1:A:230:ILE:HD12	1:A:261:THR:CG2	2.13	0.73
1:C:225:LYS:HD2	1:C:227:ILE:CD1	2.17	0.73
1:C:352:GLN:HB2	1:C:365:LEU:HD11	1.68	0.73
1:E:183:LEU:HD13	1:E:384:ALA:CB	2.18	0.73
1:G:223:ALA:HB3	1:G:252:GLU:H	1.54	0.73
1:C:256:GLY:HA3	1:C:259:LEU:HD12	1.69	0.73
1:G:264:VAL:O	1:G:267:MET:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:PHE:HB2	1:G:282:GLY:HA2	1.70	0.73
1:A:13:ARG:NH1	7:A:773:HOH:O	2.21	0.73
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.71	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:F:39:VAL:HG21	1:G:16:MET:CE	2.18	0.72
1:G:226:LYS:H	1:G:227:ILE:HG13	1.53	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:E:82:ASN:ND2	7:E:743:HOH:O	2.23	0.72
1:G:222:LEU:HD13	1:G:300:VAL:HG13	1.72	0.72
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.71	0.71
1:G:176:THR:CG2	1:G:378:VAL:HG22	2.19	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:A:266:THR:HA	1:A:270:ILE:HG22	1.72	0.71
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.71	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:E:169:VAL:HG13	1:E:173:GLY:HA3	1.73	0.71
1:G:383:ALA:HB1	1:G:388:GLU:HG2	1.72	0.71
1:A:207:LYS:HG3	1:A:214:GLU:HG3	1.72	0.70
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.73	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:F:218:PRO:HA	1:F:246:PRO:HG2	1.72	0.70
1:G:223:ALA:HB3	1:G:252:GLU:N	2.06	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:A:304:GLU:OE1	1:A:304:GLU:N	2.25	0.70
1:B:181:THR:HG22	1:B:182:GLY:H	1.56	0.70
1:C:420:ILE:CD1	1:C:451:LEU:HD13	2.22	0.70
1:C:276:VAL:HG11	1:C:325:ILE:HD13	1.73	0.70
1:C:252:GLU:OE2	1:C:285:ARG:NH2	2.25	0.69
1:C:310:GLU:N	1:C:310:GLU:OE1	2.24	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:D:265:ASN:HB3	1:D:270:ILE:HG23	1.72	0.69
1:G:225:LYS:HB3	1:G:226:LYS:CG	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:183:LEU:CD1	1:G:384:ALA:HB3	2.22	0.69
1:G:217:SER:N	1:G:218:PRO:HD3	2.07	0.69
1:G:268:ARG:NH1	1:G:270:ILE:HB	2.06	0.69
1:B:18:ARG:HD2	7:B:781:HOH:O	1.92	0.69
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.08	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:B:232:GLU:HA	1:B:310:GLU:HG2	1.75	0.69
1:F:204:PHE:HB3	1:F:266:THR:HG21	1.72	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:D:194:GLN:O	1:D:371:LYS:HE3	1.93	0.68
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.76	0.68
1:F:239:ALA:HB1	1:F:314:LEU:HD21	1.75	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:A:183:LEU:HD23	1:A:383:ALA:HB1	1.75	0.68
1:G:223:ALA:HB1	1:G:224:ASP:C	2.14	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: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:G:221:LEU:HD23	1:G:317:LEU:HG	1.75	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:A:518:GLU:HG2	7:G:730:HOH:O	1.96	0.66
1:C:353:ILE:HG12	1:C:365:LEU:CD2	2.26	0.66
1:F:268:ARG:HA	1:F:268:ARG:HE	1.60	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:G:197:ALA:HB3	1:G:330:THR:CG2	2.25	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:D:187:LEU:HD23	1:D:379:ILE:HG12	1.77	0.65
1:F:268:ARG:HA	1:F:268:ARG:NE	2.10	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:A:381:VAL:HG11	1:A:392:LYS:HB3	1.79	0.65
1:E:207:LYS:HZ3	1:E:210:THR:HG21	1.60	0.65
1:F:131:LEU:HD21	1:F:500:THR:HG22	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: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:B:319:GLN:HB2	1:B:336:VAL:HG21	1.79	0.64
1:G:222:LEU:HD11	1:G:301:ILE:H	1.61	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:A:220:ILE:HD12	1:A:296:THR:HG21	1.78	0.64
1:C:325:ILE:CD1	1:C:326:ASN:H	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:HB3	7:A:740:HOH:O	1.97	0.64
1:C:219:PHE:CD1	1:C:317:LEU:HD11	2.33	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:E:301:ILE:HG21	1:E:309:LEU:HD23	1.79	0.63
1:G:367:GLU:O	1:G:371:LYS:HG2	1.98	0.63
1:E:266:THR:OG1	1:E:273:VAL:HG12	1.98	0.63
1:F:301:ILE:HD11	1:F:308:GLU:N	2.13	0.63
1:A:104:LEU:HB3	5:A:605:MPD:HM1	1.81	0.63
1:C:227:ILE:HG22	1:C:233:MET:HE1	1.80	0.63
1:B:209:GLU:HG2	1:B:210:THR:N	2.14	0.63
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.80	0.63
1:D:225:LYS:HD2	1:D:303:GLU:HG2	1.80	0.63
1:F:39:VAL:HG21	1:G:16:MET:HE1	1.79	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:358:SER:HB3	1:F:361:ASP:HB2	1.80	0.63
1:B:513:LEU:O	1:B:517:THR:HG23	1.98	0.63
1:E:247:LEU:HB3	1:E:273:VAL:HG23	1.80	0.63
1:E:445:ARG:NH1	5:E:604:MPD:HM1	2.14	0.63
1:F:221:LEU:HB3	1:F:249:ILE:HD12	1.79	0.63
1:G:278:ALA:CB	1:G:279:PRO:HD2	2.20	0.63
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.80	0.63
1:C:215:LEU:HD13	1:C:218:PRO:CG	2.28	0.63
1:D:160:LYS:NZ	1:D:164:GLU:OE2	2.23	0.63
1:G:222:LEU:CD2	1:G:300:VAL:HG22	2.29	0.63
1:A:310:GLU:N	1:A:310:GLU:OE1	2.32	0.62
1:B:229:ASN:ND2	1:B:231:ARG:HB2	2.13	0.62
1:D:165:ALA:O	1:D:169:VAL:HG22	1.99	0.62
1:E:215:LEU:HB2	1:E:323:VAL:CG2	2.29	0.62
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.98	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:D:463:SER:HB2	7:D:740:HOH:O	1.99	0.62
1:F:248:LEU:HD13	1:F:325:ILE:HD11	1.81	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:D:400:LEU:O	1:D:404:ARG:HG2	2.00	0.61
1:G:319:GLN:HB3	1:G:336:VAL:CG2	2.29	0.61
1:A:284:ARG:HD3	1:A:364:LYS:NZ	2.15	0.61
1:G:279:PRO:CB	1:G:285:ARG:HB2	2.30	0.61
1:A:302:SER:HB2	1:A:305:ILE:CG1	2.30	0.61
1:C:346:VAL:O	1:C:350:ARG:HG2	2.00	0.61
1:G:291:ASP:HB3	1:G:372:LEU:HD11	1.81	0.61
1:G:218:PRO:HG2	1:G:323:VAL:HG22	1.81	0.61
1:F:231:ARG:HG3	1:F:231:ARG:HH11	1.65	0.61
1:G:392:LYS:NZ	7:G:737:HOH:O	2.34	0.61
1:B:198:GLY:H	1:B:277:LYS:HE3	1.66	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:G:261:THR:O	1:G:264:VAL:HG13	2.01	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: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:G:197:ALA:HA	1:G:277:LYS:HG2	1.84	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:A:34:LYS:HG3	1:A:458:CYS:SG	2.42	0.60
1:G:222:LEU:HD21	1:G:300:VAL:HA	1.83	0.60
1:B:268:ARG:NH1	1:B:268:ARG:HG2	2.18	0.59
1:E:253:ASP:OD1	1:E:254:VAL:N	2.35	0.59
1:G:284:ARG:NH1	1:G:284:ARG:HG3	2.08	0.59
1:A:270:ILE:HG23	1:A:271:VAL:C	2.22	0.59
1:C:215:LEU:CD1	1:C:323:VAL:HB	2.24	0.59
1:E:207:LYS:HZ2	1:E:210:THR:HG21	1.65	0.59
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASP:HA	1:D:389:MET:HE1	1.83	0.59
1:F:227:ILE:HD12	1:F:309:LEU:HD21	1.83	0.59
1:G:200:LEU:HD13	1:G:254:VAL:HG22	1.85	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: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:276:VAL:HG23	1:G:278:ALA:H	1.67	0.59
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.32	0.59
1:C:253:ASP:OD1	1:C:254:VAL:N	2.35	0.59
1:G:221:LEU:CD2	1:G:317:LEU:HG	2.33	0.59
1:G:30:THR:HB	1:G:51:LYS:O	2.03	0.59
1:B:264:VAL:O	1:B:268:ARG:HG3	2.03	0.59
1:E:39:VAL:HG21	1:F:16:MET:HE1	1.84	0.59
1:A:198:GLY:HA3	1:A:327:LYS:O	2.03	0.59
1:B:39:VAL:HG21	1:C:16:MET:CE	2.31	0.59
1:B:420:ILE:HD13	1:B:448:GLU:HG2	1.85	0.59
1:D:200:LEU:HD12	1:D:254:VAL:HB	1.84	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:G:250:ILE:HG13	1:G:251:ALA:N	2.15	0.59
1:D:308:GLU:CB	1:D:311:LYS:HE3	2.33	0.58
1:G:301:ILE:HG12	1:G:307:MET:HG2	1.85	0.58
1:A:242:LYS:CE	1:B:229:ASN:HB2	2.33	0.58
1:E:194:GLN:O	1:E:371:LYS:HE3	2.03	0.58
1:G:154:SER:HB3	7:G:716:HOH:O	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
1:A:282:GLY:O	1:A:286:LYS:HG2	2.03	0.58
5:G:604:MPD:H51	7:G:748:HOH:O	2.04	0.58
1:C:192:GLY:HA2	1:C:295:LEU:HD21	1.86	0.58
1:A:284:ARG:CZ	1:A:364:LYS:HG2	2.34	0.58
1:C:16:MET:HG3	1:C:520:MET:HE1	1.85	0.58
1:D:149:THR:O	1:D:154:SER:N	2.35	0.58
1:F:213:VAL:HG12	1:F:214:GLU:N	2.18	0.58
1:G:197:ALA:HB3	1:G:330:THR:HG21	1.85	0.58
1:B:178:GLU:HA	1:B:393:LYS:HE3	1.86	0.58
1:C:353:ILE:CG1	1:C:365:LEU:HD22	2.33	0.58
1:E:389:MET:CE	1:E:390:LYS:HD2	2.22	0.58
1:C:10:ASN:O	1:C:14:VAL:HG23	2.04	0.58
1:C:200:LEU:CD1	1:C:254:VAL:HG23	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:SER:OG	1:C:361:ASP:OD2	2.21	0.58
1:D:235:PRO:HG2	1:D:310:GLU:HA	1.85	0.58
1:E:205:ILE:HD12	1:E:211:GLY:HA2	1.85	0.58
1:E:197:ALA:HB1	1:E:276:VAL:HB	1.85	0.58
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:C:179:ASP:HB3	1:C:389:MET:CE	2.33	0.58
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.86	0.58
7:C:733:HOH:O	1:D:518:GLU:HG2	2.02	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
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:G:248:LEU:HD21	1:G:250:ILE:HG23	1.85	0.57
1:A:420:ILE:HD13	1:A:448:GLU:HG2	1.86	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:B:347:ALA:O	1:B:351:GLN:HG2	2.04	0.57
1:F:250:ILE:HG22	1:F:289:LEU:HD21	1.85	0.57
1:G:299:THR:HB	1:G:316:ASP:OD1	2.04	0.57
1:A:285:ARG:O	1:A:289:LEU:HG	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:287:ALA:HB1	1:A:368:ARG:NH1	2.19	0.57
1:C:265:ASN:O	1:C:270:ILE:HG12	2.05	0.57
1:D:388:GLU:O	1:D:392:LYS:N	2.31	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:136:VAL:HG13	1:D:137:PRO:HD2	1.85	0.57
1:G:230:ILE:CG2	1:G:258:ALA:HA	2.35	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:226:LYS:N	1:G:227:ILE:HG13	2.18	0.57
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.86	0.57
1:G:187:LEU:HD13	1:G:379:ILE:CG2	2.35	0.57
1:B:169:VAL:HG23	1:B:173:GLY:HA3	1.87	0.56
1:B:209:GLU:HG2	1:B:210:THR:H	1.70	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:B:215:LEU:CD2	1:B:272:LYS:HG3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLY:HA2	5:B:608:MPD:H12	1.86	0.56
1:C:251:ALA:O	1:C:278:ALA:N	2.38	0.56
1:C:401:HIS:HB2	7:C:760:HOH:O	2.05	0.56
1:C:69:MET:O	1:C:73:MET:HG3	2.05	0.56
1:A:220:ILE:CD1	1:A:296:THR:HG21	2.35	0.56
1:C:215:LEU:HD12	1:C:215:LEU:O	2.05	0.56
1:D:209:GLU:N	1:D:209:GLU:OE1	2.27	0.56
1:D:225:LYS:HB2	1:D:303:GLU:CG	2.36	0.56
1:E:89:THR:HB	7:E:743:HOH:O	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: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:395:ARG:HG3	1:G:396:VAL:N	2.21	0.56
1:G:199:TYR:HE1	1:G:202:PRO:HG3	1.71	0.56
1:D:243:ALA:O	1:E:231:ARG:NH1	2.38	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:G:257:GLU:HG2	1:G:261:THR:HB	1.86	0.56
1:B:277:LYS:HD2	1:B:277:LYS:O	2.06	0.56
1:C:317:LEU:O	1:C:317:LEU:HD12	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:B:214:GLU:OE1	1:B:322:ARG:NH2	2.38	0.55
1:C:325:ILE:HD12	1:C:329:THR:O	2.06	0.55
1:F:177:VAL:CG1	1:F:397:GLU:HG2	2.36	0.55
1:F:498:LYS:HG3	1:F:501:ARG:HH21	1.70	0.55
1:G:281:PHE:CB	1:G:285:ARG:HD3	2.36	0.55
1:B:234:LEU:HA	1:B:237:LEU:HD12	1.87	0.55
1:F:204:PHE:CB	1:F:266:THR:HG21	2.37	0.55
1:G:281:PHE:CD2	1:G:282:GLY:HA2	2.40	0.55
1:E:445:ARG:HH12	5:E:604:MPD:HM1	1.70	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: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
7:A:751:HOH:O	1:B:518:GLU:HG2	2.05	0.55
1:C:230:ILE:HG22	1:C:258:ALA:CB	2.35	0.55
1:C:77:VAL:HG13	1:C:506:TYR:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:MET:HG2	1:E:295:LEU:CD2	2.37	0.55
1:F:215:LEU:HB2	1:F:323:VAL:CG2	2.29	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:D:128:VAL:HG12	1:D:132:LYS:HE3	1.89	0.55
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.07	0.55
1:C:260:ALA:O	1:C:263:VAL:HG13	2.07	0.55
1:F:160:LYS:HE2	1:F:164:GLU:OE2	2.06	0.55
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.89	0.55
1:B:178:GLU:HB2	1:B:322:ARG:NH1	2.22	0.55
1:B:392:LYS:HE3	7:B:806:HOH:O	2.06	0.55
1:E:7:LYS:HD2	1:E:11:ASP:OD1	2.07	0.55
1:G:221:LEU:HD12	1:G:249:ILE:HG12	1.88	0.55
1:A:193:MET:HG3	1:A:371:LYS:HB3	1.89	0.54
1:C:150:ILE:HB	7:C:787:HOH:O	2.07	0.54
1:C:213:VAL:HG13	1:C:325:ILE:HG23	1.88	0.54
1:F:342:ILE:O	1:F:346:VAL:HG23	2.07	0.54
1:G:205:ILE:HG23	1:G:212:ALA:O	2.06	0.54
1:G:85:ALA:HB1	1:G:499:VAL:HG22	1.89	0.54
1:C:294:THR:HG23	1:C:341:ALA:HB1	1.87	0.54
1:G:365:LEU:HD12	1:G:366:GLN:N	2.22	0.54
1:A:179:ASP:OD1	1:A:393:LYS:HD2	2.08	0.54
1:B:10:ASN:O	1:B:14:VAL:HG13	2.07	0.54
1:G:209:GLU:HG2	1:G:210:THR:N	2.22	0.54
1:G:229:ASN:ND2	1:G:231:ARG:HB2	2.21	0.54
1:G:281:PHE:HB2	1:G:282:GLY:O	2.08	0.54
1:A:263:VAL:O	1:A:266:THR:OG1	2.25	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:F:248:LEU:CD1	1:F:325:ILE:HD11	2.38	0.54
1:G:278:ALA:HB1	1:G:279:PRO:CD	2.33	0.54
1:G:218:PRO:HG2	1:G:323:VAL:CG2	2.37	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:A:162:ILE:HG22	1:A:166:MET:CE	2.37	0.54
1:A:267:MET:HB2	1:A:268:ARG:HH21	1.73	0.54
1:B:34:LYS:HE2	1:C:118[A]:ARG:NH2	2.22	0.54
1:F:200:LEU:HD12	1:F:254:VAL:HB	1.89	0.54
1:F:232:GLU:CD	1:F:309:LEU:HD13	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:PRO:HB2	1:G:285:ARG:CB	2.33	0.54
1:B:441:LYS:HE2	7:B:812:HOH:O	2.08	0.54
1:G:200:LEU:HD12	1:G:275:ALA:HB1	1.89	0.54
1:A:177:VAL:HG11	1:A:397:GLU:HG3	1.89	0.54
1:C:215:LEU:HD13	1:C:218:PRO:HG3	1.90	0.54
1:F:445[B]:ARG:NH2	7:F:720:HOH:O	2.40	0.54
1:A:200:LEU:CD1	1:A:254:VAL:HB	2.38	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:C:39:VAL:HG12	1:D:69:MET:CE	2.38	0.54
1:C:82:ASN:HB2	1:C:89:THR:OG1	2.08	0.54
1:D:310:GLU:OE1	1:D:310:GLU:N	2.30	0.54
1:D:463:SER:O	1:D:467:ASN:HB2	2.08	0.54
1:C:305:ILE:CG2	1:C:307:MET:HG3	2.38	0.53
1:C:325:ILE:HG13	1:C:326:ASN:N	2.23	0.53
1:E:203:TYR:O	1:E:267:MET:HE2	2.07	0.53
1:G:384:ALA:O	1:G:385:THR:OG1	2.24	0.53
1:A:184:GLN:OE1	1:A:184:GLN:N	2.32	0.53
1:C:199:TYR:HE1	1:C:202:PRO:HA	1.70	0.53
1:C:385:THR:HG22	1:C:386:GLU:N	2.23	0.53
1:F:288:MET:O	1:F:292:ILE:HG13	2.08	0.53
1:F:302:SER:O	1:F:307:MET:HB2	2.08	0.53
1:F:30:THR:HB	1:F:51:LYS:O	2.08	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:G:281:PHE:HB2	1:G:282:GLY:C	2.29	0.53
1:B:229:ASN:HD21	1:B:231:ARG:HB2	1.73	0.53
1:C:120:ILE:O	1:C:124:VAL:HG23	2.07	0.53
1:E:232:GLU:HG2	1:E:310:GLU:OE2	2.07	0.53
1:E:383:ALA:HB1	1:E:388:GLU:HB2	1.91	0.53
1:A:223:ALA:HB3	1:A:251:ALA:HB2	1.89	0.53
1:B:14:VAL:HG12	5:B:604:MPD:H51	1.90	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:A:136:VAL:HG13	1:A:137:PRO:HD2	1.89	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:G:221:LEU:HB2	1:G:249:ILE:HG23	1.91	0.53
1:G:224:ASP:OD2	1:G:302:SER:HB2	2.08	0.53
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.09	0.53
1:B:359:ASP:OD1	1:B:362:ARG:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:HG12	5:B:604:MPD:C5	2.39	0.53
1:F:231:ARG:HD2	1:F:231:ARG:O	2.08	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:D:193:MET:CE	1:D:371:LYS:HD3	2.39	0.53
1:F:221:LEU:HA	1:F:317:LEU:HD23	1.90	0.53
1:G:187:LEU:HD13	1:G:379:ILE:HG23	1.91	0.53
1:B:217:SER:HB3	1:B:245:LYS:NZ	2.24	0.52
1:B:86:GLY:CA	5:B:608:MPD:H12	2.40	0.52
1:C:276:VAL:HG11	1:C:325:ILE:CD1	2.37	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:A:381:VAL:HG21	1:A:393:LYS:CA	2.37	0.52
1:A:77:VAL:HG13	1:A:506:TYR:HB3	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:C:243:ALA:HB3	1:C:244:GLY:CA	2.39	0.52
1:C:281:PHE:HA	1:C:285:ARG:HD3	1.91	0.52
1:E:2:ALA:HB3	7:E:751:HOH:O	2.08	0.52
1:B:177:VAL:CG1	1:B:397:GLU:HG3	2.39	0.52
1:B:263:VAL:HG22	1:B:267:MET:CE	2.40	0.52
1:B:301:ILE:HD13	1:B:312:ALA:HB2	1.91	0.52
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.91	0.52
1:D:230:ILE:HG21	1:D:261:THR:HG21	1.91	0.52
1:G:273:VAL:HG12	1:G:274:ALA:N	2.23	0.52
1:D:236:VAL:O	1:D:240:VAL:HG23	2.10	0.52
1:G:171:LYS:HD3	1:G:407:VAL:HG13	1.91	0.52
1:A:169:VAL:CG1	1:A:173:GLY:HA3	2.40	0.52
1:B:16:MET:HE2	1:B:73:MET:SD	2.50	0.52
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.90	0.52
1:C:227:ILE:HG22	1:C:233:MET:HE3	1.92	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:C:248:LEU:CD2	1:C:323:VAL:HG11	2.37	0.52
1:C:259:LEU:CA	1:C:262:LEU:HD13	2.40	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:F:10:ASN:O	1:F:14:VAL:HG13	2.09	0.52
1:G:171:LYS:HD3	1:G:407:VAL:CG1	2.39	0.52
1:G:227:ILE:N	1:G:227:ILE:HD12	2.24	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:A:77:VAL:HG21	1:A:510:VAL:HB	1.92	0.52
1:C:222:LEU:CB	1:C:300:VAL:HG23	2.35	0.52
1:C:417:VAL:HG21	1:C:488:MET:HG3	1.92	0.52
1:D:38:VAL:HG22	1:E:519:CYS:HB3	1.92	0.52
1:G:222:LEU:O	1:G:222:LEU:HD12	2.09	0.52
1:A:271:VAL:HG23	1:A:272:LYS:HD3	1.91	0.51
1:B:30:THR:HB	1:B:51:LYS:O	2.09	0.51
1:G:197:ALA:HA	1:G:277:LYS:CG	2.40	0.51
1:G:193:MET:HB2	1:G:371:LYS:HB3	1.92	0.51
1:A:397:GLU:O	1:A:401:HIS:ND1	2.32	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:C:194:GLN:O	1:C:371:LYS:HE3	2.09	0.51
1:C:256:GLY:CA	1:C:259:LEU:HB2	2.39	0.51
1:G:285:ARG:HG2	1:G:286:LYS:N	2.24	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:A:291:ASP:OD2	1:A:368:ARG:HD2	2.10	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:E:193:MET:CE	1:E:372:LEU:HD12	2.40	0.51
1:F:265:ASN:HA	1:F:268:ARG:HB2	1.93	0.51
1:G:197:ALA:HB3	1:G:330:THR:HG22	1.91	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:G:268:ARG:NH1	1:G:271:VAL:HG23	2.26	0.51
1:A:39:VAL:HG21	1:B:16:MET:HE3	1.88	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:D:152:ALA:N	1:D:153:ASN:HA	2.25	0.51
1:F:209:GLU:HG2	1:F:210:THR:HG23	1.93	0.51
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.92	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:B:253:ASP:OD1	1:B:254:VAL:N	2.42	0.51
1:C:325:ILE:CG1	1:C:326:ASN:H	2.24	0.51
1:C:112:ASN:HB3	1:C:115:ASP:HB2	1.93	0.50
1:G:150:ILE:CD1	1:G:493:ILE:HA	2.41	0.50
1:C:344:GLY:O	1:C:348:GLN:HG3	2.11	0.50
1:G:120:ILE:O	1:G:124:VAL:HG23	2.11	0.50
1:G:268:ARG:CG	1:G:268:ARG:HH11	2.22	0.50
1:G:251:ALA:HB2	1:G:279:PRO:HD2	1.92	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:B:458:CYS:SG	1:B:480:ALA:HB1	2.52	0.50
1:C:364:LYS:HG3	1:C:365:LEU:N	2.27	0.50
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.77	0.50
1:F:270:ILE:O	1:F:270:ILE:HD12	2.11	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:B:77:VAL:HG13	1:B:506:TYR:HB3	1.93	0.50
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.94	0.50
1:E:366:GLN:O	1:E:369:VAL:HG22	2.12	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:A:69:MET:CE	1:G:39:VAL:HG12	2.42	0.50
1:C:219:PHE:O	1:C:247:LEU:HD12	2.11	0.50
1:C:313:THR:HG23	1:C:316:ASP:H	1.76	0.50
1:C:32:GLY:HA3	7:C:740:HOH:O	2.11	0.50
1:D:209:GLU:HG2	1:D:210:THR:N	2.26	0.50
1:D:224:ASP:O	1:D:252:GLU:HB2	2.12	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
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: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
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:C:173:GLY:O	1:C:404:ARG:NH2	2.35	0.49
1:C:229:ASN:OD1	1:C:259:LEU:HG	2.12	0.49
1:E:291:ASP:OD2	1:E:368:ARG:HD2	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:G:458:CYS:HB3	7:G:719:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:THR:HB	1:C:51:LYS:O	2.12	0.49
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:B:231:ARG:HA	1:B:234:LEU:HG	1.93	0.49
1:F:153:ASN:OD1	7:F:706:HOH:O	2.20	0.49
1:F:164:GLU:HA	1:F:167[B]:ASP:OD2	2.12	0.49
1:G:281:PHE:CB	1:G:282:GLY:HA2	2.41	0.49
1:B:259:LEU:HD12	1:B:260:ALA:H	1.76	0.49
1:C:288:MET:HA	1:C:291:ASP:HB2	1.93	0.49
1:C:217:SER:N	1:C:321:LYS:O	2.39	0.49
1:D:198:GLY:HA3	1:D:327:LYS:O	2.13	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.94	0.49
1:F:183:LEU:CD1	1:F:184:GLN:H	2.25	0.49
1:G:178:GLU:O	1:G:381:VAL:HG23	2.11	0.49
1:G:385:THR:HG22	1:G:387:VAL:H	1.77	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:E:261:THR:O	1:E:264:VAL:HB	2.12	0.49
1:F:203:TYR:HD2	1:F:263:VAL:HG13	1.76	0.49
1:B:392:LYS:HA	1:B:395:ARG:HE	1.77	0.49
1:D:128:VAL:CG1	1:D:132:LYS:HE3	2.43	0.49
1:E:383:ALA:O	1:E:384:ALA:HB3	2.13	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:C:305:ILE:HG23	1:C:307:MET:HG3	1.95	0.49
1:D:152:ALA:CB	1:D:155:ASP:H	2.25	0.49
1:B:157:THR:HB	7:B:806:HOH:O	2.13	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:E:217:SER:HA	1:E:320:ALA:O	2.12	0.49
1:F:186:GLU:HG3	1:F:187:LEU:N	2.27	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:G:171:LYS:HB3	1:G:407:VAL:HG11	1.95	0.49
1:C:202:PRO:O	1:C:203:TYR:HB2	2.13	0.49
1:C:279:PRO:HG2	1:C:288:MET:HE2	1.95	0.49
1:D:118[A]:ARG:NH2	7:D:785:HOH:O	2.46	0.49
1:D:200:LEU:CD1	1:D:254:VAL:HB	2.42	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:E:258:ALA:O	1:E:262:LEU:HD13	2.13	0.49
1:F:221:LEU:CD2	1:F:249:ILE:HD12	2.42	0.49
1:G:10:ASN:HB3	7:G:736:HOH:O	2.12	0.49
1:G:279:PRO:HB2	1:G:285:ARG:HA	1.94	0.49
1:G:24:ALA:O	1:G:28:LYS:HG2	2.12	0.49
1:B:181:THR:CG2	1:B:182:GLY:H	2.24	0.49
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.95	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:E:321:LYS:O	1:E:321:LYS:HD3	2.13	0.49
1:G:197:ALA:CA	1:G:277:LYS:HG2	2.43	0.49
1:B:225:LYS:HD2	1:B:303:GLU:OE2	2.13	0.48
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:E:215:LEU:HB2	1:E:323:VAL:HG22	1.94	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:G:493:ILE:HD13	2:G:601:ADP:C6	2.48	0.48
1:A:358:SER:HB3	1:A:361:ASP:OD2	2.13	0.48
1:B:198:GLY:N	1:B:277:LYS:HE3	2.28	0.48
1:C:215:LEU:C	1:C:215:LEU:HD12	2.33	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:D:33:PRO:HG2	1:D:480:ALA:HB3	1.94	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:G:16:MET:HE2	1:G:73:MET:SD	2.54	0.48
1:A:385:THR:HG22	1:A:386:GLU:N	2.28	0.48
1:C:225:LYS:HE2	1:C:254:VAL:HA	1.95	0.48
1:G:248:LEU:C	1:G:248:LEU:HD23	2.34	0.48
1:A:69:MET:HE2	1:G:39:VAL:HG12	1.95	0.48
1:E:403:THR:O	1:E:407:VAL:HG23	2.13	0.48
1:B:217:SER:HB3	1:B:245:LYS:HZ1	1.78	0.48
1:C:293:ALA:HB1	1:C:298:GLY:O	2.13	0.48
1:C:326:ASN:OD1	1:C:327:LYS:HG2	2.13	0.48
1:E:140:ASP:N	1:E:140:ASP:OD1	2.46	0.48
1:F:201:SER:HB2	1:F:204:PHE:HE2	1.77	0.48
1:G:124:VAL:O	1:G:128: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.49	0.48
1:B:381:VAL:CG1	1:B:392:LYS:HD3	2.43	0.48
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:F:186:GLU:CG	1:F:187:LEU:N	2.77	0.48
1:F:171:LYS:O	1:F:404:ARG:NH1	2.44	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:B:232:GLU:HA	1:B:310:GLU:CG	2.44	0.48
1:C:172:GLU:OE1	1:C:172:GLU:N	2.40	0.48
1:C:206:ASN:OD1	1:C:214:GLU:N	2.47	0.48
1:C:243:ALA:HB3	1:C:244:GLY:HA2	1.96	0.48
1:D:288:MET:O	1:D:291:ASP:HB2	2.13	0.48
1:E:386:GLU:O	1:E:390:LYS:HG2	2.14	0.48
1:G:216:GLU:OE2	1:G:321:LYS:NZ	2.47	0.48
1:C:35:GLY:O	1:C:51:LYS:HE2	2.14	0.48
1:G:222:LEU:CD2	1:G:300:VAL:HA	2.44	0.48
1:G:242:LYS:O	1:G:243:ALA:HB3	2.14	0.48
1:G:385:THR:CG2	1:G:387:VAL:HG12	2.43	0.48
1:B:263:VAL:O	1:B:267:MET:HG3	2.14	0.47
1:E:218:PRO:CB	1:E:246:PRO:HG2	2.32	0.47
1:E:383:ALA:HB2	1:E:389:MET:HA	1.95	0.47
1:F:313:THR:HG22	1:F:314:LEU:N	2.29	0.47
1:C:206:ASN:ND2	1:C:214:GLU:H	2.12	0.47
1:C:203:TYR:HB3	1:C:267:MET:SD	2.55	0.47
1:E:16:MET:HG2	1:E:514:MET:CE	2.44	0.47
1:F:217:SER:N	1:F:321:LYS:O	2.35	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:B:150:ILE:HD11	1:B:493:ILE:HA	1.97	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:A:144:ILE:CG2	1:A:166:MET:HE3	2.43	0.47
1:A:229:ASN:HB3	1:A:232:GLU:OE1	2.14	0.47
1:A:261:THR:HG23	1:A:265:ASN:ND2	2.29	0.47
1:A:381:VAL:HG13	1:A:392:LYS:HD3	1.95	0.47
1:B:34:LYS:HE2	1:C:118[A]:ARG:HH22	1.79	0.47
1:B:38:VAL:HG22	1:C:519:CYS:HB3	1.97	0.47
1:E:264:VAL:O	1:E:268:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:PHE:HB3	1:F:266:THR:OG1	2.13	0.47
1:F:225:LYS:NZ	1:F:308:GLU:HA	2.29	0.47
1:F:345:ARG:O	1:F:349:ILE:HG13	2.14	0.47
1:G:257:GLU:HG2	1:G:261:THR:OG1	2.15	0.47
1:G:281:PHE:HB3	1:G:285:ARG:HD3	1.96	0.47
1:A:242:LYS:HE2	1:B:229:ASN:HB2	1.96	0.47
1:C:227:ILE:HG22	1:C:228:SER:N	2.22	0.47
1:C:68:ASN:O	1:C:72:GLN:HG2	2.15	0.47
1:E:180:GLY:HA3	1:E:381:VAL:C	2.35	0.47
1:A:253:ASP:HB3	7:A:725:HOH:O	2.14	0.47
1:A:284:ARG:O	1:A:288:MET:HG3	2.15	0.47
1:B:149:THR:OG1	1:B:156:GLU:HA	2.14	0.47
1:E:417:VAL:HG21	1:E:488:MET:HG3	1.96	0.47
1:E:444:LEU:HD23	1:E:447:MET:HE1	1.96	0.47
1:F:227:ILE:CD1	1:F:309:LEU:HD21	2.44	0.47
1:B:288:MET:O	1:B:292:ILE:HG13	2.14	0.47
1:C:270:ILE:HG13	1:C:271:VAL:H	1.80	0.47
1:C:349:ILE:HG22	1:C:365:LEU:HD23	1.96	0.47
1:C:489:ILE:HD13	1:C:494:LEU:CD2	2.44	0.47
1:D:219:PHE:O	1:D:247:LEU:HD12	2.14	0.47
1:D:385:THR:HG23	1:D:388:GLU:HG2	1.97	0.47
1:G:325:ILE:N	1:G:325:ILE:HD12	2.30	0.47
1:G:15:LYS:HD3	1:G:66:PHE:HB2	1.97	0.47
1:A:108:ALA:HB2	5:A:605:MPD:HM2	1.95	0.47
1:A:266:THR:HG22	1:A:270:ILE:HG21	1.96	0.47
1:B:276:VAL:HG11	1:B:325:ILE:HD13	1.97	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:F:204:PHE:HB3	1:F:266:THR:HB	1.93	0.47
1:G:219:PHE:CB	1:G:317:LEU:HD23	2.39	0.47
1:G:222:LEU:HD11	1:G:300:VAL:CA	2.37	0.47
1:A:68:ASN:O	1:A:72:GLN:HG2	2.15	0.47
1:C:206:ASN:HD21	1:C:214:GLU:H	1.62	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: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: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
5:B:605:MPD:O4	5:B:605:MPD:HM2	2.15	0.46
1:D:257:GLU:O	1:D:261:THR:OG1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASP:O	1:F:252:GLU:HG3	2.15	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
1:G:392:LYS:O	1:G:396:VAL:HG23	2.14	0.46
1:A:349:ILE:HB	1:A:369:VAL:HG12	1.96	0.46
1:A:381:VAL:CG1	1:A:392:LYS:HD3	2.45	0.46
1:D:445:ARG:NH2	7:D:730:HOH:O	2.48	0.46
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.15	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: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: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:F:215:LEU:HB3	1:F:218:PRO:HB3	1.97	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:B:227:ILE:CD1	1:B:309:LEU:HD22	2.46	0.46
1:C:200:LEU:CD1	1:C:254:VAL:CG2	2.94	0.46
1:C:261:THR:HA	1:C:264:VAL:CG1	2.45	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:F:165:ALA:O	1:F:169:VAL:HG22	2.16	0.46
1:F:222:LEU:O	1:F:301:ILE:HG22	2.15	0.46
1:G:205:ILE:HA	1:G:213:VAL:CG2	2.45	0.46
1:G:105:LYS:HG2	5:G:604:MPD:O4	2.14	0.46
1:A:498:LYS:NZ	5:A:609:MPD:H53	2.31	0.46
1:B:227:ILE:HD12	1:B:309:LEU:CD2	2.46	0.46
1:C:231:ARG:NH1	1:C:258:ALA:HB1	2.31	0.46
1:C:348:GLN:O	1:C:352:GLN:HG3	2.15	0.46
1:C:385:THR:HG22	1:C:386:GLU:H	1.81	0.46
1:E:219:PHE:CE2	1:E:245:LYS:HD3	2.51	0.46
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.56	0.46
1:F:381:VAL:CG2	1:F:392:LYS:HD3	2.45	0.46
1:A:270:ILE:CG2	1:A:271:VAL:C	2.84	0.46
1:D:166:MET:HG2	1:D:175:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:444:LEU:CA	1:E:447:MET:HE3	2.39	0.46
1:F:264:VAL:O	1:F:268:ARG:HB2	2.16	0.46
1:G:264:VAL:HG22	1:G:265:ASN:N	2.30	0.46
1:A:169:VAL:HG23	1:A:377:ALA:HB2	1.97	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:C:227:ILE:CG2	1:C:233:MET:HE3	2.46	0.46
1:G:221:LEU:O	1:G:250:ILE:HG12	2.16	0.46
1:G:268:ARG:HH22	1:G:271:VAL:CG2	2.29	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:B:363:GLU:O	1:B:367:GLU:HG3	2.15	0.45
1:D:253:ASP:OD1	1:D:254:VAL:N	2.49	0.45
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.98	0.45
1:G:247:LEU:HD12	1:G:248:LEU:H	1.81	0.45
1:A:224:ASP:OD1	1:A:286:LYS:HD2	2.17	0.45
1:C:243:ALA:HB3	1:C:245:LYS:N	2.31	0.45
1:C:265:ASN:ND2	1:C:270:ILE:HD11	2.31	0.45
1:F:14:VAL:O	1:F:18[B]:ARG:HG3	2.16	0.45
1:G:301:ILE:HG23	1:G:307:MET:CG	2.44	0.45
1:G:321:LYS:HZ2	1:G:322:ARG:HB2	1.81	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:F:242:LYS:O	1:G:257:GLU:HB2	2.17	0.45
1:G:281:PHE:CB	1:G:282:GLY:CA	2.86	0.45
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.98	0.45
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.99	0.45
1:A:38:VAL:HG22	1:B:519:CYS:HB3	1.99	0.45
1:D:226:LYS:HD2	1:D:255:GLU:CD	2.37	0.45
1:D:385:THR:HG22	1:D:388:GLU:HG2	1.96	0.45
1:G:385:THR:HB	1:G:388:GLU:CB	2.41	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:B:215:LEU:HB3	1:B:218:PRO:HB3	1.99	0.45
1:C:308:GLU:O	1:C:311:LYS:HB3	2.17	0.45
1:E:193:MET:HE1	1:E:372:LEU:HD12	1.99	0.45
1:E:102:GLU:HB2	1:E:442:VAL:HG13	1.98	0.45
1:E:19:GLY:HA3	1:E:67:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ILE:N	1:G:220:ILE:HD12	2.32	0.45
1:A:366:GLN:O	1:A:369:VAL:HG22	2.16	0.45
1:C:231:ARG:HH12	1:C:258:ALA:HB1	1.82	0.45
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.41	0.45
1:G:192:GLY:HA2	1:G:295:LEU:HD21	1.99	0.45
1:G:350:ARG:O	1:G:353:ILE:HG12	2.17	0.45
1:B:248:LEU:HD13	1:B:325:ILE:HD11	1.99	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:100:ILE:HD13	1:G:514:MET:SD	2.56	0.45
1:G:155:ASP:HB3	1:G:158:VAL:CG1	2.46	0.45
1:G:215:LEU:HB2	1:G:218:PRO:HG2	1.97	0.45
1:G:262:LEU:O	1:G:262:LEU:HD12	2.17	0.45
1:B:188:ASP:N	1:B:188:ASP:OD1	2.49	0.45
1:B:227:ILE:HG21	1:B:233:MET:CE	2.38	0.45
1:C:200:LEU:CD1	1:C:254:VAL:HB	2.47	0.45
1:D:270:ILE:O	1:D:270:ILE:HG12	2.17	0.45
1:D:273:VAL:HG22	1:D:274:ALA:N	2.32	0.45
1:D:392:LYS:O	1:D:395:ARG:HB3	2.16	0.45
1:F:25:ASP:OD1	1:F:28:LYS:HE2	2.16	0.45
1:G:277:LYS:O	1:G:278:ALA:HB3	2.16	0.45
1:G:104:LEU:HB3	5:G:604:MPD:H12	1.99	0.45
1:G:68:ASN:O	1:G:72:GLN:HG2	2.17	0.45
1:A:230:ILE:O	1:A:230:ILE:HG12	2.16	0.44
1:B:140:ASP:OD2	1:B:142:LYS:HB3	2.16	0.44
1:C:259:LEU:HA	1:C:262:LEU:CD1	2.44	0.44
1:C:179:ASP:HB3	1:C:389:MET:HE3	1.98	0.44
1:F:225:LYS:HZ2	1:F:309:LEU:HD12	1.82	0.44
1:F:177:VAL:HG13	1:F:397:GLU:HG2	1.98	0.44
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.99	0.44
1:A:344:GLY:O	1:A:348:GLN:HG3	2.17	0.44
1:A:401:HIS:O	1:A:404:ARG:HB2	2.16	0.44
1:B:455:VAL:HG21	1:B:465:VAL:HG11	1.98	0.44
1:C:198:GLY:HA3	1:C:327:LYS:O	2.17	0.44
1:C:213:VAL:CG1	1:C:325:ILE:HG23	2.47	0.44
1:F:235:PRO:HG3	1:F:310:GLU:CA	2.48	0.44
1:A:124:VAL:O	1:A:128:VAL:HG23	2.17	0.44
1:A:16:MET:HB3	1:A:16:MET:HE2	1.84	0.44
1:A:456:LEU:HG	5:A:608:MPD:H12	2.00	0.44
1:A:475:ASN:O	1:A:488:MET:HG2	2.17	0.44
1:C:259:LEU:C	1:C:262:LEU:HD13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ASP:O	1:C:29:VAL:HG13	2.17	0.44
1:C:352:GLN:HA	1:C:355:GLU:CD	2.38	0.44
1:G:285:ARG:HG3	1:G:289:LEU:HD12	2.00	0.44
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.17	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:B:181:THR:CG2	1:B:182:GLY:N	2.81	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:309:LEU:N	1:F:309:LEU:HD12	2.32	0.44
1:F:420:ILE:HD13	1:F:448:GLU:HG2	1.99	0.44
1:G:268:ARG:HH22	1:G:271:VAL:HG23	1.82	0.44
1:C:230:ILE:HG21	1:C:258:ALA:HB1	1.98	0.44
1:C:456:LEU:HD13	1:C:462:PRO:HG2	1.99	0.44
1:D:136:VAL:HG13	1:D:137:PRO:CD	2.47	0.44
1:A:498:LYS:HZ1	5:A:609:MPD:H53	1.82	0.44
1:B:260:ALA:HA	1:B:263:VAL:CG1	2.48	0.44
1:C:219:PHE:CG	1:C:245:LYS:HD2	2.53	0.44
1:D:152:ALA:HB3	1:D:154:SER:N	2.33	0.44
5:D:605:MPD:H11	5:D:605:MPD:O4	2.17	0.44
1:F:225:LYS:HZ2	1:F:308:GLU:HA	1.83	0.44
1:F:391:GLU:HG2	1:F:392:LYS:N	2.33	0.44
1:G:385:THR:HG21	1:G:387:VAL:HG12	2.00	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:D:325:ILE:N	1:D:325:ILE:HD12	2.32	0.44
1:E:219:PHE:HE2	1:E:245:LYS:HD3	1.83	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:G:225:LYS:HA	1:G:226:LYS:HA	1.50	0.44
1:A:348:GLN:O	1:A:352:GLN:HG3	2.18	0.44
1:D:336:VAL:O	1:D:336:VAL:HG12	2.18	0.44
1:E:117:LYS:NZ	7:E:750:HOH:O	2.51	0.44
1:F:186:GLU:CD	1:F:187:LEU:H	2.22	0.44
1:F:349:ILE:O	1:F:353:ILE:HG12	2.18	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
5:A:608:MPD:HM1	1:B:518:GLU:HG3	2.00	0.44
1:D:326:ASN:OD1	1:D:329:THR:N	2.46	0.44
1:D:389:MET:HG3	1:D:390:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:CD1	1:E:254:VAL:HB	2.47	0.44
1:E:201:SER:HA	1:E:202:PRO:HD3	1.89	0.44
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: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
2:E:601:ADP:O2A	2:E:601:ADP:O1B	2.36	0.43
1:E:81:ALA:HB1	7:E:719:HOH:O	2.17	0.43
1:G:18[A]:ARG:HG2	1:G:67:GLU:CD	2.38	0.43
1:B:361:ASP:O	1:B:365:LEU:HD13	2.18	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:F:313:THR:HG22	1:F:314:LEU:H	1.84	0.43
1:B:205:ILE:HG22	1:B:207:LYS:H	1.83	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: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:G:16:MET:HB3	1:G:514:MET:CE	2.49	0.43
1:C:301:ILE:HD11	1:C:312:ALA:CB	2.48	0.43
1:D:363:GLU:O	1:D:367:GLU:HG3	2.19	0.43
1:E:219:PHE:HB3	1:E:317:LEU:HD23	2.00	0.43
1:G:392:LYS:HE3	1:G:395:ARG:HH21	1.84	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:F:215:LEU:HD12	1:F:323:VAL:HG21	2.00	0.43
1:G:251:ALA:CB	1:G:289:LEU:HD21	2.47	0.43
1:A:393:LYS:NZ	1:A:397:GLU:OE2	2.38	0.43
1:B:362:ARG:O	1:B:366:GLN:HB2	2.18	0.43
1:A:37:ASN:CB	1:B:517:THR:HG22	2.49	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:D:302:SER:O	1:D:307:MET:HB2	2.19	0.43
1:F:246:PRO:CB	1:F:272:LYS:HE3	2.46	0.43
1:G:27:VAL:HG12	1:G:90:THR:HG23	2.00	0.43
1:B:359:ASP:O	1:B:363:GLU:HG3	2.18	0.43
1:B:15:LYS:NZ	1:B:64:ASP:OD2	2.49	0.43
1:C:172:GLU:H	1:C:172:GLU:CD	2.22	0.43
1:D:176:THR:CG2	1:D:378:VAL:HG22	2.49	0.43
1:D:385:THR:O	1:D:389:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:LYS:O	1:E:164:GLU:HG3	2.19	0.43
1:A:162:ILE:HG22	1:A:166:MET:HE1	2.00	0.43
1:C:219:PHE:CD2	1:C:245:LYS:HD2	2.53	0.43
1:C:200:LEU:HD12	1:C:254:VAL:HB	2.01	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:F:230:ILE:O	1:F:234:LEU:HG	2.19	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: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:C:272:LYS:HD2	1:C:272:LYS:N	2.34	0.42
1:C:434:GLU:HG2	7:C:763:HOH:O	2.19	0.42
1:D:177:VAL:HG12	1:D:393:LYS:HG3	2.00	0.42
1:F:160:LYS:O	1:F:164:GLU:HG3	2.18	0.42
1:F:221:LEU:CB	1:F:249:ILE:HD12	2.47	0.42
1:G:219:PHE:HE1	1:G:245:LYS:HD3	1.83	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:F:185:ASP:N	1:F:185:ASP:OD1	2.39	0.42
1:G:321:LYS:HB3	1:G:334:ASP:HB3	2.00	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:A:106:ALA:O	1:A:111:MET:HG3	2.19	0.42
1:A:363:GLU:O	1:A:367:GLU:HG3	2.19	0.42
1:A:169:VAL:CG2	1:A:377:ALA:HB2	2.48	0.42
1:B:222:LEU:HD22	1:B:289:LEU:HD22	2.00	0.42
1:C:225:LYS:HZ3	1:C:259:LEU:CD2	2.32	0.42
1:D:152:ALA:HB1	1:D:155:ASP:HB3	2.00	0.42
1:E:339:GLU:O	1:E:343:GLN:HG2	2.20	0.42
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.19	0.42
1:F:232:GLU:OE1	1:F:309:LEU:HD13	2.19	0.42
1:F:417:VAL:O	1:F:421:ARG:HG2	2.19	0.42
1:G:264:VAL:HG22	1:G:265:ASN:ND2	2.34	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:C:227:ILE:CG2	1:C:228:SER:H	2.16	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:E:383:ALA:HB1	1:E:388:GLU:CB	2.50	0.42
1:G:251:ALA:CB	1:G:279:PRO:HD2	2.50	0.42
1:A:195:PHE:CE1	1:A:330:THR:HB	2.55	0.42
1:B:268:ARG:HH11	1:B:268:ARG:CG	2.29	0.42
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.83	0.42
1:C:456:LEU:HD13	1:C:462:PRO:CG	2.50	0.42
1:D:14:VAL:O	1:D:18[B]:ARG:HG3	2.19	0.42
1:D:222:LEU:HD23	1:D:250:ILE:HB	2.01	0.42
1:D:232:GLU:OE2	1:D:309:LEU:HD12	2.19	0.42
1:F:349:ILE:HG21	1:F:369:VAL:HG13	2.01	0.42
1:A:272:LYS:HB2	1:A:272:LYS:HE2	1.92	0.42
1:C:207:LYS:O	1:C:207:LYS:HG3	2.20	0.42
1:C:226:LYS:HD3	1:C:252:GLU:OE2	2.19	0.42
1:D:143:ALA:O	1:D:147:VAL:HG23	2.20	0.42
1:D:266:THR:HA	1:D:271:VAL:HG13	2.02	0.42
1:G:183:LEU:HA	1:G:384:ALA:HB2	2.02	0.42
1:A:391:GLU:O	1:A:394:ALA:HB3	2.20	0.42
1:C:206:ASN:O	1:C:207:LYS:HG2	2.19	0.42
1:C:215:LEU:HD11	1:C:323:VAL:N	2.35	0.42
1:C:266:THR:OG1	1:C:271:VAL:O	2.25	0.42
1:G:279:PRO:HG2	1:G:285:ARG:HB2	2.01	0.42
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.60	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:F:367:GLU:O	1:F:371:LYS:HG3	2.20	0.42
1:A:325:ILE:N	1:A:325:ILE:HD12	2.35	0.42
1:C:256:GLY:HA3	1:C:259:LEU:HB2	2.01	0.42
1:C:27:VAL:HG12	1:C:90:THR:HG23	2.01	0.42
1:D:187:LEU:HD13	1:D:187:LEU:C	2.40	0.42
1:D:366:GLN:O	1:D:369:VAL:HG22	2.19	0.42
1:D:417:VAL:HG21	1:D:477:GLY:HA3	2.01	0.42
1:E:263:VAL:O	1:E:263:VAL:HG12	2.20	0.42
1:F:232:GLU:HG3	1:F:309:LEU:HD22	2.02	0.42
1:G:187:LEU:HD13	1:G:379:ILE:HG22	2.02	0.42
1:G:230:ILE:HA	1:G:233:MET:HG2	2.02	0.42
1:G:46:ALA:HA	1:G:47:PRO:HD3	1.84	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:B:217:SER:HA	1:B:320:ALA:O	2.19	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:350:ARG:HA	1:F:353:ILE:HG13	2.02	0.41
1:F:501:ARG:HG2	1:F:505:GLN:OE1	2.20	0.41
1:G:352:GLN:HA	1:G:355:GLU:CB	2.38	0.41
1:B:220:ILE:CD1	1:B:296:THR:HG21	2.50	0.41
1:C:209:GLU:HG2	1:C:210:THR:N	2.35	0.41
1:C:217:SER:O	1:C:245:LYS:HG3	2.20	0.41
1:E:184:GLN:HA	1:E:184:GLN:OE1	2.20	0.41
1:F:183:LEU:N	1:F:183:LEU:HD12	2.35	0.41
1:G:219:PHE:CE1	1:G:245:LYS:HD3	2.55	0.41
1:C:16:MET:SD	1:C:73:MET:HE1	2.60	0.41
1:D:16:MET:HG3	1:D:520:MET:SD	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:G:360:TYR:CE2	1:G:364:LYS:HE2	2.55	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:E:49:ILE:CD1	1:F:513:LEU:HD13	2.50	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:A:266:THR:CG2	1:A:270:ILE:HG21	2.50	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:C:215:LEU:CD1	1:C:323:VAL:H	2.33	0.41
1:C:393:LYS:NZ	1:C:397:GLU:OE2	2.53	0.41
1:D:39:VAL:HG12	1:E:69:MET:CE	2.51	0.41
1:F:364:LYS:HD3	1:F:367:GLU:OE1	2.21	0.41
7:E:745:HOH:O	1:F:518:GLU:HG2	2.18	0.41
1:A:270:ILE:CD1	1:A:273:VAL:HB	2.36	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:C:215:LEU:HD11	1:C:218:PRO:HG3	2.02	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:D:183:LEU:HD12	1:D:183:LEU:N	2.36	0.41
1:E:342:ILE:O	1:E:346:VAL:HG23	2.19	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:A:234:LEU:N	1:A:235:PRO:HD2	2.36	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:A:514:MET:HE2	1:A:514:MET:HB3	1.66	0.41
1:B:259:LEU:HD12	1:B:260:ALA:CA	2.51	0.41
1:D:227:ILE:HG22	1:D:258:ALA:CB	2.50	0.41
1:F:310:GLU:H	1:F:310:GLU:CD	2.21	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:A:177:VAL:HG11	1:A:397:GLU:CG	2.49	0.41
1:A:281:PHE:N	1:A:285:ARG:HB2	2.36	0.41
1:A:46:ALA:HA	1:A:47:PRO:HD3	1.93	0.41
1:B:234:LEU:N	1:B:235:PRO:HD2	2.35	0.41
1:B:287:ALA:HB1	1:B:368:ARG:NH1	2.36	0.41
1:C:256:GLY:O	1:C:260:ALA:N	2.53	0.41
1:E:366:GLN:HG2	7:E:742:HOH:O	2.20	0.41
1:A:131:LEU:CD1	1:A:422:VAL:HG21	2.43	0.41
1:D:68:ASN:O	1:D:72:GLN:HG2	2.21	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: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:C:350:ARG:O	1:C:353:ILE:HB	2.20	0.41
1:D:160:LYS:HG2	1:D:164:GLU:OE2	2.21	0.41
1:G:284:ARG:NH1	1:G:364:LYS:HE3	2.35	0.41
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.51	0.41
1:F:193:MET:HB2	1:F:371:LYS:HB3	2.03	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:G:461:GLU:HA	1:G:462:PRO:HD3	1.84	0.41
1:A:222:LEU:O	1:A:301:ILE:HG22	2.21	0.40
1:A:162:ILE:HD11	1:A:399:ALA:HB3	2.03	0.40
1:C:259:LEU:O	1:C:262:LEU:HD13	2.21	0.40
1:D:381:VAL:HG12	1:D:382:GLY:N	2.36	0.40
1:D:455:VAL:HG21	1:D:465:VAL:HG11	2.03	0.40
1:D:524:LEU:HA	1:D:525:PRO:HD3	1.97	0.40
1:E:124:VAL:O	1:E:128:VAL:HG23	2.21	0.40
1:E:381:VAL:CG2	1:E:392:LYS:HD3	2.51	0.40
1:F:308:GLU:HB3	1:F:310:GLU:OE2	2.20	0.40
1:A:225:LYS:HD2	1:A:303:GLU:OE1	2.21	0.40
1:A:30:THR:HB	1:A:51:LYS:O	2.21	0.40
1:C:273:VAL:HG22	1:C:274:ALA:N	2.35	0.40
1:C:364:LYS:O	1:C:367:GLU:HB2	2.21	0.40
1:C:420:ILE:HD12	1:C:451:LEU:CD1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:604:MPD:O4	5:D:604:MPD:H12	2.21	0.40
1:E:163:ALA:O	1:E:167:ASP:HB2	2.22	0.40
1:E:33:PRO:HG3	2:E:601:ADP:C6	2.55	0.40
1:F:231:ARG:HG3	1:F:231:ARG:NH1	2.33	0.40
1:F:234:LEU:N	1:F:235:PRO:CD	2.82	0.40
1:F:326:ASN:HB3	1:F:329:THR:HB	2.02	0.40
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.21	0.40
1:C:39:VAL:HG12	1:D:69:MET:HE2	2.03	0.40
1:C:455:VAL:O	1:C:458:CYS:HB2	2.21	0.40
1:D:193:MET:HB2	1:D:193:MET:HE2	1.92	0.40
1:E:22:VAL:HG11	1:E:62:LEU:HD21	2.02	0.40
1:E:365:LEU:CD2	1:E:368:ARG:HH21	2.34	0.40
1:G:165:ALA:O	1:G:169:VAL:HG22	2.21	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: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:G:226:LYS:HB2	1:G:227:ILE:CA	2.44	0.40
1:B:222:LEU:HD22	1:B:289:LEU:CD2	2.52	0.40
1:B:16:MET:HG3	1:B:520:MET:CE	2.52	0.40
1:B:5:ASP:HB2	1:B:524:LEU:HD23	2.04	0.40
1:C:229:ASN:HA	1:C:259:LEU:CD1	2.51	0.40
1:D:381:VAL:HG12	1:D:392:LYS:HD3	2.04	0.40
1:D:420:ILE:CD1	1:D:448:GLU:HG2	2.51	0.40
1:F:314:LEU:HA	1:F:317:LEU:HD12	2.03	0.40
1:F:77:VAL:HG21	1:F:510:VAL:HB	2.03	0.40
1:G:204:PHE:HB3	1:G:213:VAL:HG21	2.02	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

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	523/548 (95%)	512 (98%)	11 (2%)	0	100	100
1	B	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	47	72
1	C	525/548 (96%)	505 (96%)	19 (4%)	1 (0%)	47	72
1	D	524/548 (96%)	509 (97%)	15 (3%)	0	100	100
1	E	523/548 (95%)	512 (98%)	10 (2%)	1 (0%)	47	72
1	F	526/548 (96%)	512 (97%)	13 (2%)	1 (0%)	47	72
1	G	523/548 (95%)	502 (96%)	21 (4%)	0	100	100
All	All	3667/3836 (96%)	3561 (97%)	102 (3%)	4 (0%)	51	77

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

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%)	41	69
1	B	403/413 (98%)	395 (98%)	8 (2%)	55	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	405/413 (98%)	393 (97%)	12 (3%)	41	69
1	D	404/413 (98%)	392 (97%)	12 (3%)	41	69
1	E	403/413 (98%)	390 (97%)	13 (3%)	39	67
1	F	406/413 (98%)	397 (98%)	9 (2%)	52	78
1	G	403/413 (98%)	385 (96%)	18 (4%)	27	53
All	All	2827/2891 (98%)	2743 (97%)	84 (3%)	42	69

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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	24,29,29	0.95	1 (4%)	29,45,45	1.43	4 (13%)
5	MPD	D	606	-	7,7,7	0.43	0	9,10,10	0.69	0
5	MPD	C	604	-	7,7,7	0.41	0	9,10,10	0.81	0
5	MPD	G	604	-	7,7,7	0.36	0	9,10,10	0.53	0
5	MPD	B	604	-	7,7,7	0.39	0	9,10,10	0.43	0
2	ADP	B	601	3,4	24,29,29	1.04	2 (8%)	29,45,45	1.47	4 (13%)
5	MPD	G	605	-	7,7,7	0.80	0	9,10,10	0.92	0
5	MPD	D	604	-	7,7,7	0.33	0	9,10,10	0.30	0
2	ADP	C	601	3,4	24,29,29	0.96	1 (4%)	29,45,45	1.38	5 (17%)
5	MPD	F	604	-	7,7,7	0.32	0	9,10,10	0.47	0
2	ADP	F	601	3,4	24,29,29	0.98	1 (4%)	29,45,45	1.46	3 (10%)
5	MPD	A	607	-	7,7,7	0.34	0	9,10,10	0.35	0
5	MPD	D	605	-	7,7,7	0.32	0	9,10,10	0.52	0
5	MPD	B	606	-	7,7,7	0.38	0	9,10,10	0.52	0
2	ADP	E	601	3,4	24,29,29	0.96	1 (4%)	29,45,45	1.41	3 (10%)
5	MPD	B	608	-	7,7,7	0.37	0	9,10,10	0.42	0
5	MPD	A	609	-	7,7,7	0.24	0	9,10,10	0.48	0
5	MPD	E	604	-	7,7,7	0.38	0	9,10,10	0.50	0
5	MPD	A	608	-	7,7,7	0.32	0	9,10,10	0.77	0
2	ADP	D	601	3,4	24,29,29	0.97	2 (8%)	29,45,45	1.51	5 (17%)
5	MPD	A	606	-	7,7,7	0.37	0	9,10,10	0.75	0
5	MPD	A	605	-	7,7,7	0.37	0	9,10,10	0.63	0
2	ADP	G	601	3,4	24,29,29	1.03	2 (8%)	29,45,45	1.51	5 (17%)
5	MPD	B	607	-	7,7,7	0.31	0	9,10,10	0.44	0
5	MPD	A	604	-	7,7,7	0.41	0	9,10,10	0.36	0
5	MPD	B	605	-	7,7,7	0.32	0	9,10,10	0.61	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	-	2/12/32/32	0/3/3/3
5	MPD	D	606	-	-	3/5/5/5	-
5	MPD	C	604	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	G	604	-	-	0/5/5/5	-
5	MPD	B	604	-	-	1/5/5/5	-
2	ADP	B	601	3,4	-	6/12/32/32	0/3/3/3
5	MPD	G	605	-	-	0/5/5/5	-
5	MPD	D	604	-	-	2/5/5/5	-
2	ADP	C	601	3,4	-	2/12/32/32	0/3/3/3
5	MPD	F	604	-	-	2/5/5/5	-
2	ADP	F	601	3,4	-	7/12/32/32	0/3/3/3
5	MPD	A	607	-	-	0/5/5/5	-
5	MPD	D	605	-	-	0/5/5/5	-
5	MPD	B	606	-	-	0/5/5/5	-
2	ADP	E	601	3,4	-	6/12/32/32	0/3/3/3
5	MPD	B	608	-	-	3/5/5/5	-
5	MPD	A	609	-	-	2/5/5/5	-
5	MPD	E	604	-	-	2/5/5/5	-
5	MPD	A	608	-	-	5/5/5/5	-
2	ADP	D	601	3,4	-	2/12/32/32	0/3/3/3
5	MPD	A	606	-	-	1/5/5/5	-
5	MPD	A	605	-	-	2/5/5/5	-
2	ADP	G	601	3,4	-	3/12/32/32	0/3/3/3
5	MPD	B	607	-	-	2/5/5/5	-
5	MPD	A	604	-	-	0/5/5/5	-
5	MPD	B	605	-	-	2/5/5/5	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	2.37	1.47	1.40
2	F	601	ADP	C5-C4	2.35	1.47	1.40
2	G	601	ADP	C2-N3	2.31	1.35	1.32
2	G	601	ADP	C5-C4	2.31	1.47	1.40
2	E	601	ADP	C5-C4	2.28	1.47	1.40
2	A	601	ADP	C5-C4	2.22	1.46	1.40
2	D	601	ADP	C5-C4	2.20	1.46	1.40
2	D	601	ADP	O4'-C1'	2.15	1.44	1.41
2	C	601	ADP	C5-C4	2.14	1.46	1.40
2	B	601	ADP	C2-N3	2.12	1.35	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	PA-O3A-PB	-3.99	119.13	132.83
2	A	601	ADP	N3-C2-N1	-3.73	122.85	128.68
2	E	601	ADP	PA-O3A-PB	-3.64	120.32	132.83
2	E	601	ADP	N3-C2-N1	-3.64	122.98	128.68
2	F	601	ADP	PA-O3A-PB	-3.56	120.59	132.83
2	F	601	ADP	N3-C2-N1	-3.55	123.13	128.68
2	G	601	ADP	PA-O3A-PB	-3.48	120.89	132.83
2	C	601	ADP	N3-C2-N1	-3.43	123.31	128.68
2	D	601	ADP	N3-C2-N1	-3.42	123.34	128.68
2	B	601	ADP	N3-C2-N1	-3.08	123.86	128.68
2	D	601	ADP	C1'-N9-C4	-3.06	121.27	126.64
2	D	601	ADP	PA-O3A-PB	-3.05	122.35	132.83
2	G	601	ADP	N6-C6-N1	2.94	124.69	118.57
2	A	601	ADP	PA-O3A-PB	-2.78	123.27	132.83
2	B	601	ADP	C4-C5-N7	-2.66	106.62	109.40
2	E	601	ADP	C4-C5-N7	-2.65	106.64	109.40
2	G	601	ADP	N3-C2-N1	-2.64	124.55	128.68
2	D	601	ADP	C4-C5-N7	-2.57	106.72	109.40
2	F	601	ADP	C4-C5-N7	-2.47	106.82	109.40
2	G	601	ADP	C4-C5-N7	-2.44	106.85	109.40
2	C	601	ADP	C4-C5-N7	-2.36	106.94	109.40
2	A	601	ADP	C4-C5-N7	-2.34	106.96	109.40
2	B	601	ADP	C1'-N9-C4	-2.28	122.63	126.64
2	C	601	ADP	O2A-PA-O1A	2.09	122.59	112.24
2	C	601	ADP	N6-C6-N1	2.09	122.92	118.57
2	A	601	ADP	O2A-PA-O1A	2.07	122.47	112.24
2	C	601	ADP	C1'-N9-C4	-2.03	123.08	126.64
2	G	601	ADP	O4'-C1'-C2'	-2.01	103.98	106.93
2	D	601	ADP	O2A-PA-O1A	2.00	122.15	112.24

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	604	MPD	C2-C3-C4-C5
5	B	604	MPD	C2-C3-C4-C5
2	B	601	ADP	PA-O3A-PB-O2B
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
5	D	604	MPD	C2-C3-C4-C5
2	F	601	ADP	PA-O3A-PB-O2B
2	F	601	ADP	C5'-O5'-PA-O3A
2	F	601	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	E	601	ADP	PA-O3A-PB-O2B
2	E	601	ADP	C5'-O5'-PA-O1A
2	E	601	ADP	C5'-O5'-PA-O2A
5	A	606	MPD	C2-C3-C4-C5
5	B	605	MPD	C2-C3-C4-O4
2	E	601	ADP	C3'-C4'-C5'-O5'
2	F	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	PA-O3A-PB-O1B
2	A	601	ADP	PB-O3A-PA-O1A
2	E	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	PA-O3A-PB-O2B
2	B	601	ADP	C5'-O5'-PA-O3A
2	A	601	ADP	PB-O3A-PA-O2A
2	D	601	ADP	PB-O3A-PA-O2A
5	A	608	MPD	C2-C3-C4-C5
5	A	605	MPD	C2-C3-C4-C5
5	B	605	MPD	C2-C3-C4-C5
2	F	601	ADP	C5'-O5'-PA-O1A
5	E	604	MPD	C2-C3-C4-O4
5	A	608	MPD	C2-C3-C4-O4
5	D	606	MPD	C1-C2-C3-C4
5	D	606	MPD	CM-C2-C3-C4
5	B	608	MPD	C1-C2-C3-C4
5	A	608	MPD	C1-C2-C3-C4
5	A	608	MPD	CM-C2-C3-C4
2	B	601	ADP	C3'-C4'-C5'-O5'
2	D	601	ADP	PB-O3A-PA-O1A
2	G	601	ADP	PB-O3A-PA-O1A
2	G	601	ADP	PB-O3A-PA-O2A
2	G	601	ADP	PA-O3A-PB-O1B
5	D	606	MPD	O2-C2-C3-C4
5	B	608	MPD	O2-C2-C3-C4
5	A	608	MPD	O2-C2-C3-C4
2	B	601	ADP	PA-O3A-PB-O3B
2	F	601	ADP	PA-O3A-PB-O3B
2	E	601	ADP	C5'-O5'-PA-O3A
5	F	604	MPD	C2-C3-C4-C5
5	A	609	MPD	C2-C3-C4-C5
5	E	604	MPD	C2-C3-C4-C5
5	B	607	MPD	C2-C3-C4-C5
2	F	601	ADP	PA-O3A-PB-O1B
5	C	604	MPD	C2-C3-C4-O4

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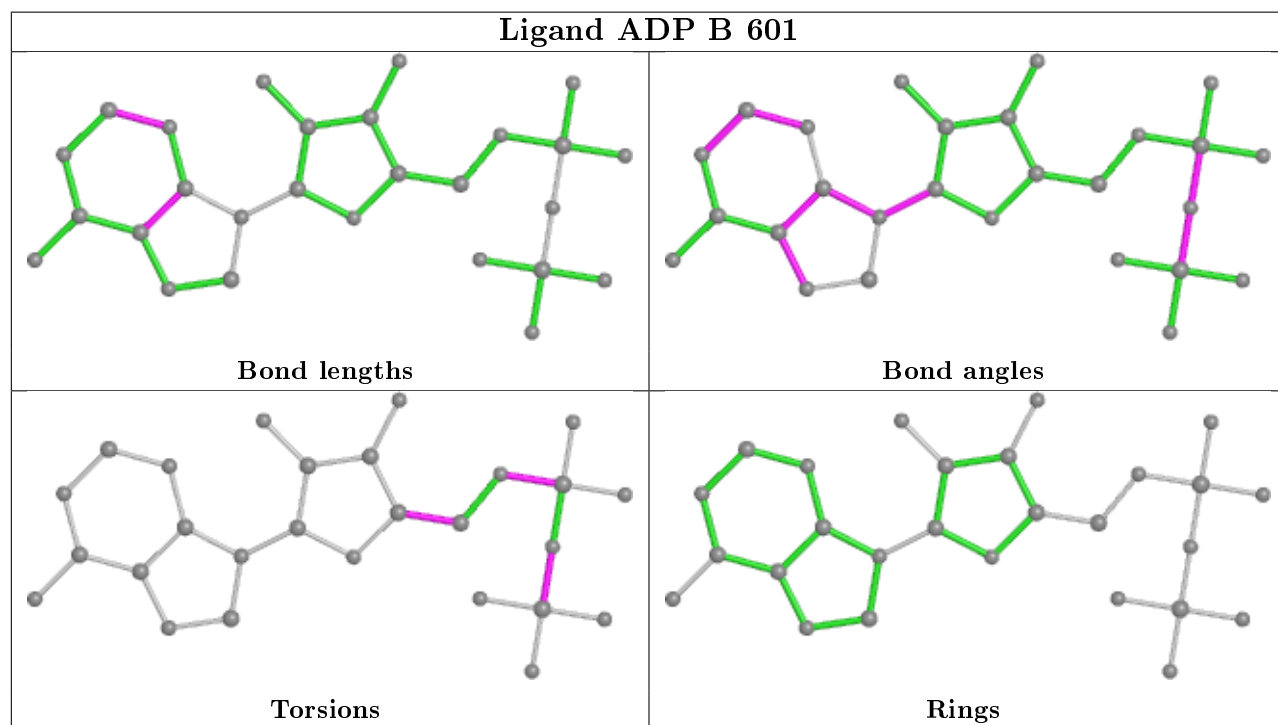
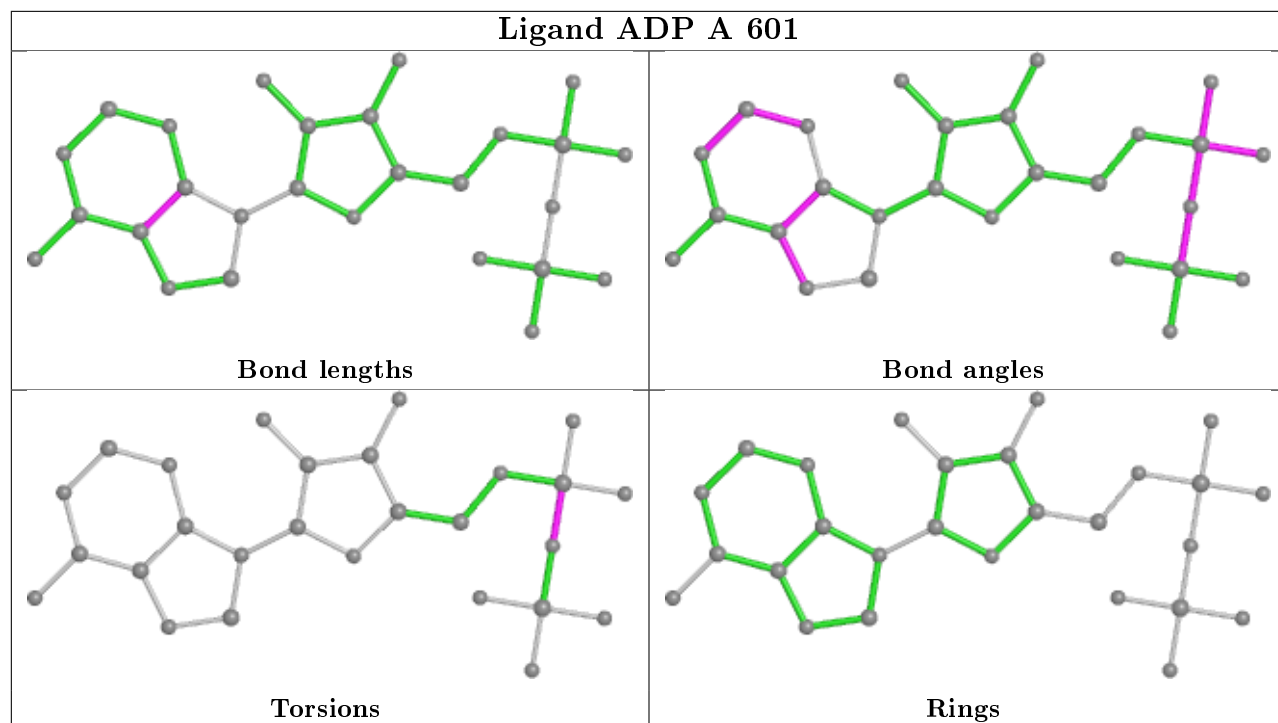
Mol	Chain	Res	Type	Atoms
5	D	604	MPD	C2-C3-C4-O4
5	F	604	MPD	C2-C3-C4-O4
5	B	608	MPD	C2-C3-C4-O4
5	A	609	MPD	C2-C3-C4-O4
5	A	605	MPD	C2-C3-C4-O4
5	B	607	MPD	C2-C3-C4-O4

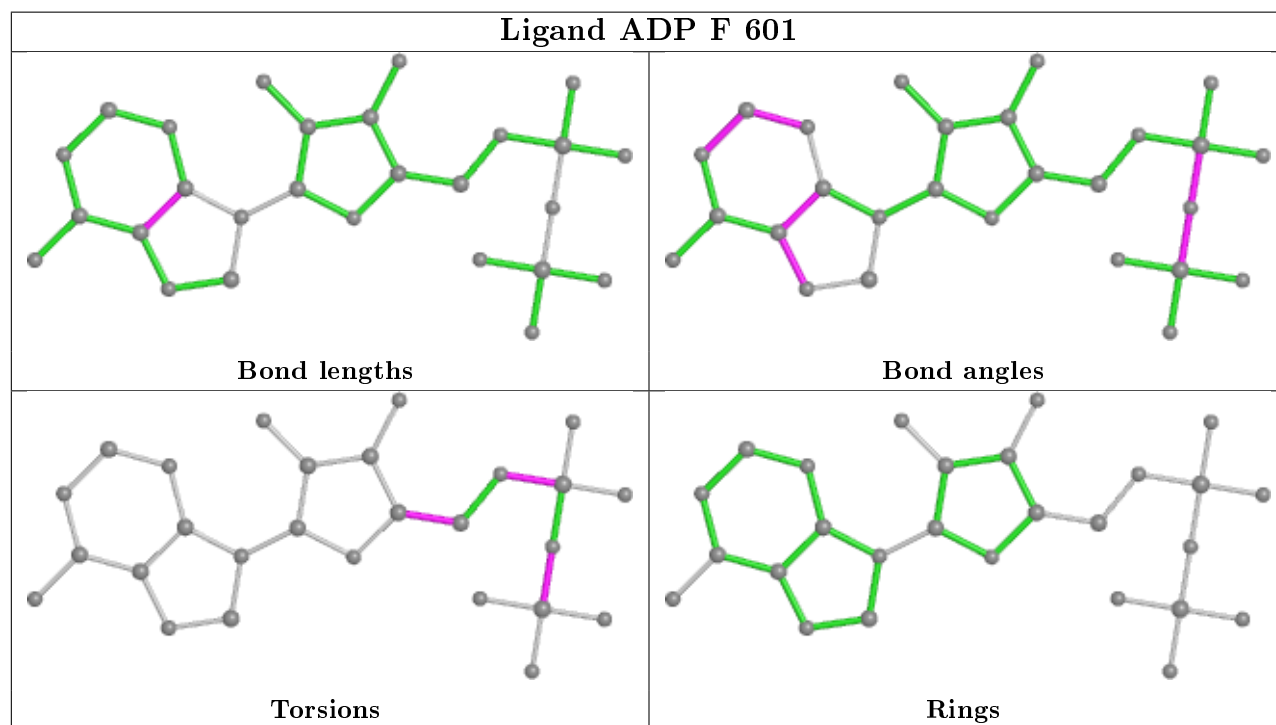
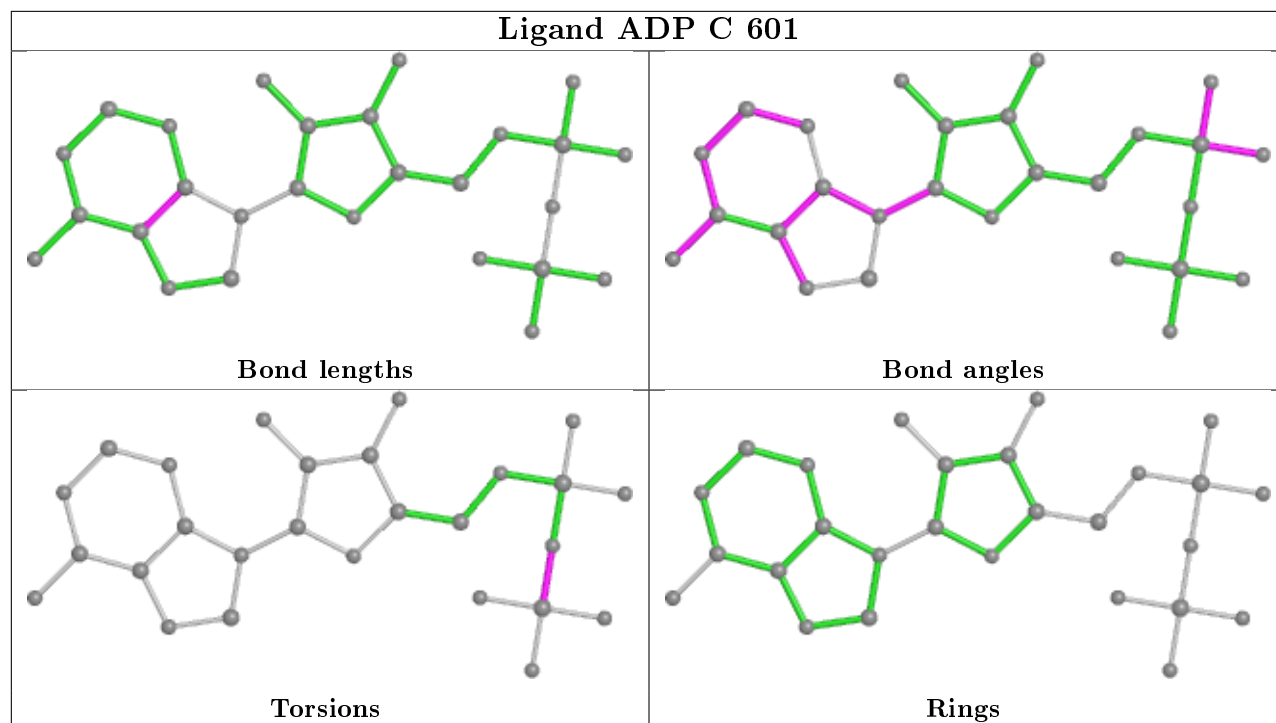
There are no ring outliers.

15 monomers are involved in 29 short contacts:

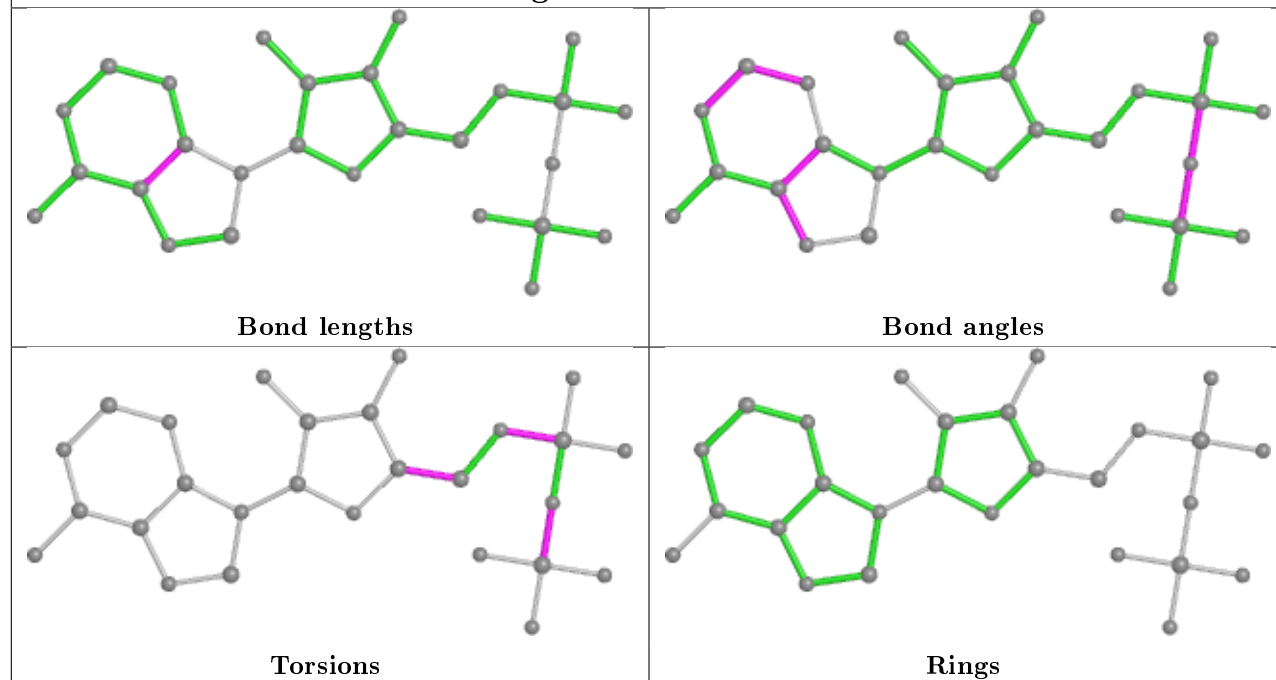
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	604	MPD	1	0
5	G	604	MPD	3	0
5	B	604	MPD	2	0
5	D	604	MPD	1	0
5	D	605	MPD	1	0
2	E	601	ADP	2	0
5	B	608	MPD	2	0
5	A	609	MPD	4	0
5	E	604	MPD	2	0
5	A	608	MPD	3	0
5	A	606	MPD	3	0
5	A	605	MPD	2	0
2	G	601	ADP	1	0
5	A	604	MPD	1	0
5	B	605	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

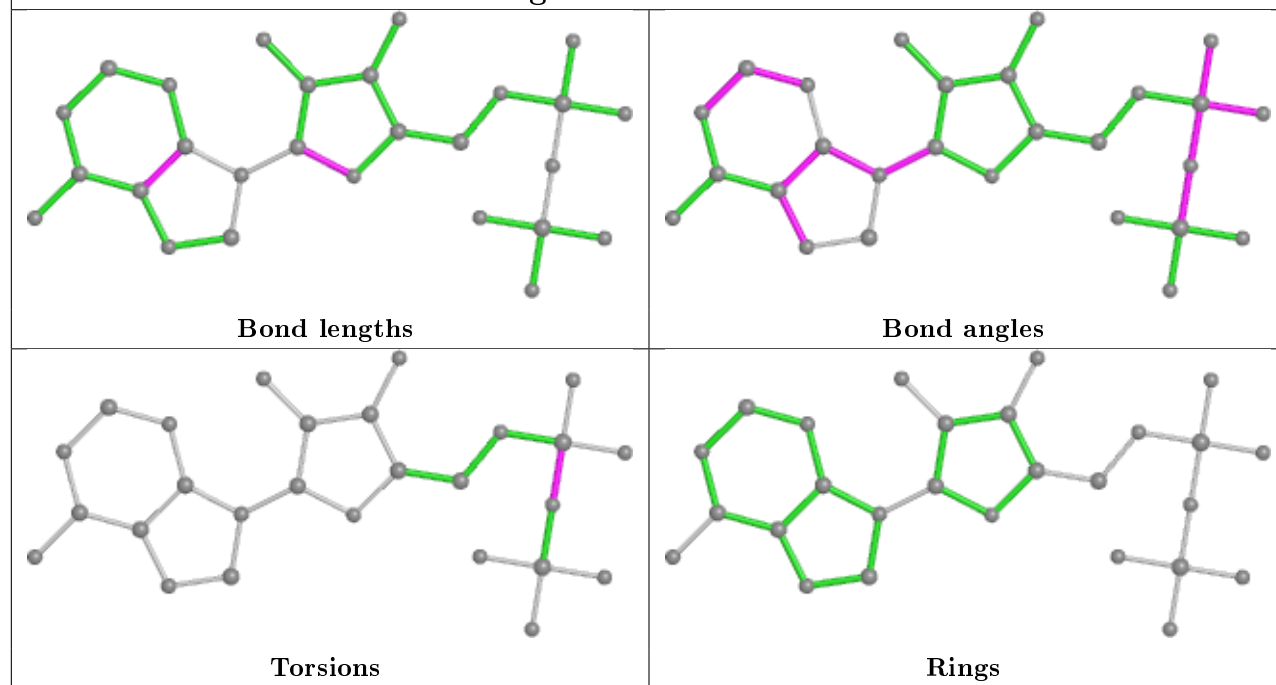


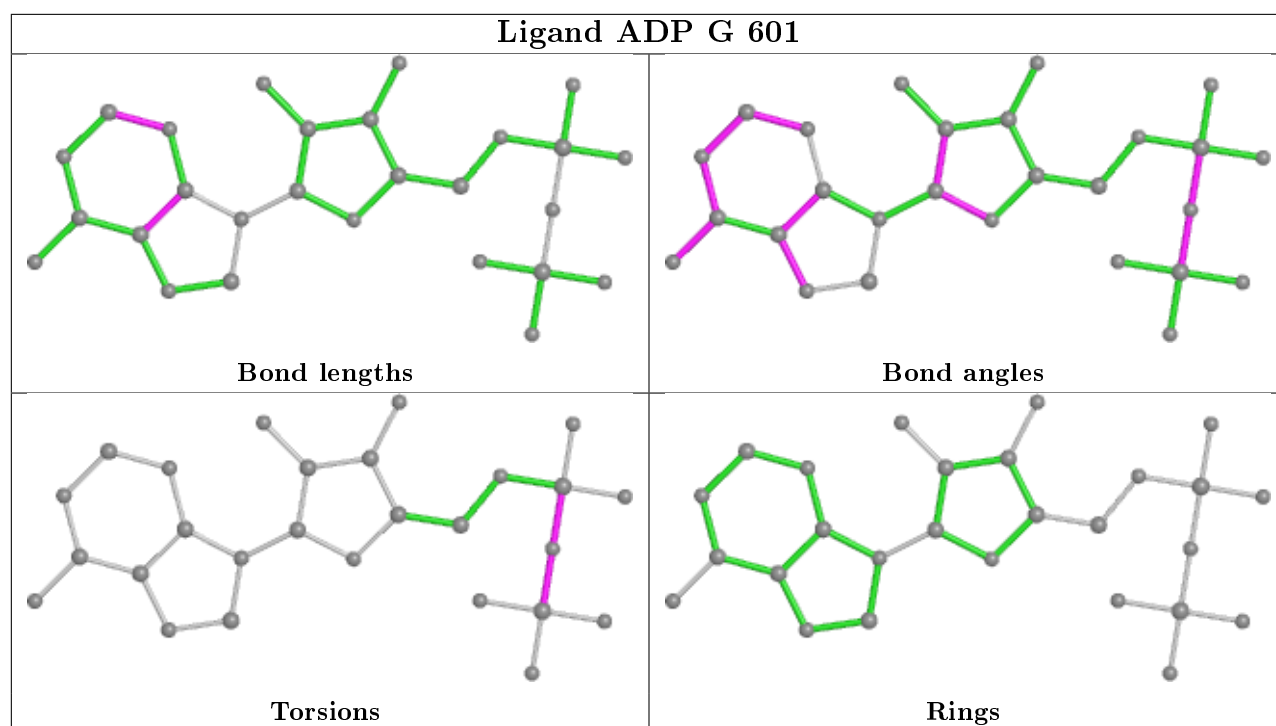


Ligand ADP E 601



Ligand ADP D 601





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	524/548 (95%)	0.03	18 (3%)	45	45	27, 69, 168, 196	0
1	B	524/548 (95%)	0.03	22 (4%)	36	35	24, 60, 160, 190	0
1	C	524/548 (95%)	0.37	65 (12%)	4	3	26, 68, 202, 243	0
1	D	524/548 (95%)	-0.13	9 (1%)	70	72	30, 71, 155, 181	0
1	E	524/548 (95%)	-0.05	13 (2%)	57	59	31, 79, 141, 187	0
1	F	524/548 (95%)	0.06	34 (6%)	18	18	33, 75, 178, 223	0
1	G	524/548 (95%)	0.40	57 (10%)	5	4	30, 71, 211, 243	0
All	All	3668/3836 (95%)	0.10	218 (5%)	22	21	24, 72, 181, 243	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	225	LYS	9.8
1	G	251	ALA	8.5
1	G	233	MET	8.1
1	E	271	VAL	8.1
1	G	301	ILE	7.3
1	G	223	ALA	7.1
1	C	309	LEU	6.9
1	B	270	ILE	6.6
1	G	203	TYR	6.2
1	G	286	LYS	6.1
1	C	307	MET	6.1
1	C	212	ALA	5.7
1	C	250	ILE	5.5
1	G	247	LEU	5.4
1	G	181	THR	5.4
1	A	271	VAL	5.2
1	C	243	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	271	VAL	5.1
1	G	226	LYS	5.0
1	G	271	VAL	4.9
1	F	347	ALA	4.9
1	C	249	ILE	4.8
1	C	236	VAL	4.8
1	F	266	THR	4.8
1	C	305	ILE	4.8
1	G	266	THR	4.7
1	C	203	TYR	4.6
1	C	244	GLY	4.6
1	G	361	ASP	4.5
1	C	226	LYS	4.5
1	G	305	ILE	4.5
1	C	240	VAL	4.5
1	F	201	SER	4.3
1	G	224	ASP	4.3
1	C	231	ARG	4.2
1	E	267	MET	4.2
1	E	383	ALA	4.2
1	C	306	GLY	4.2
1	G	314	LEU	4.2
1	G	253	ASP	4.2
1	C	383	ALA	4.1
1	C	228	SER	4.1
1	F	227	ILE	4.0
1	E	272	LYS	4.0
1	F	240	VAL	4.0
1	B	356	ALA	4.0
1	G	252	GLU	3.9
1	C	304	GLU	3.8
1	G	302	SER	3.8
1	G	387	VAL	3.8
1	G	208	PRO	3.7
1	G	308	GLU	3.7
1	C	281	PHE	3.7
1	B	360	TYR	3.6
1	F	229	ASN	3.6
1	G	204	PHE	3.6
1	A	270	ILE	3.6
1	G	250	ILE	3.6
1	C	248	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	262	LEU	3.6
1	C	232	GLU	3.6
1	A	357	THR	3.6
1	C	275	ALA	3.5
1	A	222	LEU	3.5
1	B	268	ARG	3.5
1	G	306	GLY	3.5
1	C	200	LEU	3.4
1	C	344	GLY	3.4
1	F	270	ILE	3.4
1	G	227	ILE	3.4
1	B	272	LYS	3.4
1	B	208	PRO	3.4
1	A	268	ARG	3.4
1	G	356	ALA	3.4
1	G	317	LEU	3.3
1	C	195	PHE	3.3
1	G	273	VAL	3.3
1	G	304	GLU	3.3
1	F	44	PHE	3.3
1	G	358	SER	3.2
1	C	280	GLY	3.2
1	G	281	PHE	3.2
1	C	204	PHE	3.2
1	G	277	LYS	3.2
1	C	257	GLU	3.2
1	B	340	ALA	3.1
1	G	222	LEU	3.1
1	G	315	GLU	3.1
1	C	279	PRO	3.1
1	F	233	MET	3.1
1	B	357	THR	3.1
1	E	320	ALA	3.1
1	A	349	ILE	3.1
1	C	302	SER	3.1
1	A	266	THR	3.0
1	B	271	VAL	3.0
1	G	276	VAL	3.0
1	G	258	ALA	3.0
1	G	231	ARG	3.0
1	C	208	PRO	3.0
1	C	300	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	386	GLU	3.0
1	F	259	LEU	3.0
1	G	310	GLU	3.0
1	G	379	ILE	2.9
1	B	262	LEU	2.9
1	G	300	VAL	2.9
1	D	212	ALA	2.9
1	F	200	LEU	2.9
1	C	363	GLU	2.9
1	F	239	ALA	2.9
1	C	227	ILE	2.9
1	C	253	ASP	2.9
1	C	270	ILE	2.9
1	F	260	ALA	2.8
1	B	244	GLY	2.8
1	G	249	ILE	2.8
1	F	300	VAL	2.8
1	A	336	VAL	2.8
1	B	269	GLY	2.8
1	F	204	PHE	2.8
1	C	215	LEU	2.8
1	A	305	ILE	2.8
1	E	266	THR	2.8
1	G	267	MET	2.8
1	D	267	MET	2.7
1	D	203	TYR	2.7
1	D	381	VAL	2.7
1	C	233	MET	2.7
1	F	268	ARG	2.7
1	E	203	TYR	2.7
1	B	233	MET	2.7
1	C	353	ILE	2.7
1	D	204	PHE	2.7
1	C	255	GLU	2.7
1	A	264	VAL	2.6
1	A	267	MET	2.6
1	C	359	ASP	2.6
1	B	373	ALA	2.6
1	C	254	VAL	2.6
1	C	360	TYR	2.6
1	C	315	GLU	2.6
1	E	268	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	201	SER	2.6
1	C	201	SER	2.6
1	D	44	PHE	2.5
1	F	202	PRO	2.5
1	C	269	GLY	2.5
1	F	267	MET	2.5
1	G	354	GLU	2.5
1	F	261	THR	2.5
1	F	203	TYR	2.5
1	C	237	LEU	2.5
1	F	213	VAL	2.5
1	G	313	THR	2.5
1	F	230	ILE	2.5
1	C	301	ILE	2.5
1	D	387	VAL	2.5
1	B	263	VAL	2.4
1	G	213	VAL	2.4
1	G	215	LEU	2.4
1	C	263	VAL	2.4
1	F	231	ARG	2.4
1	A	44	PHE	2.4
1	D	269	GLY	2.4
1	A	351	GLN	2.4
1	C	361	ASP	2.4
1	D	305	ILE	2.4
1	E	270	ILE	2.4
1	C	362	ARG	2.4
1	C	223	ALA	2.4
1	F	251	ALA	2.4
1	C	220	ILE	2.4
1	C	303	GLU	2.4
1	G	303	GLU	2.3
1	F	247	LEU	2.3
1	F	212	ALA	2.3
1	B	254	VAL	2.3
1	A	362	ARG	2.3
1	B	240	VAL	2.3
1	C	264	VAL	2.3
1	C	358	SER	2.3
1	B	238	GLU	2.3
1	A	353	ILE	2.3
1	C	199	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	318	GLY	2.2
1	F	301	ILE	2.2
1	C	284	ARG	2.2
1	B	223	ALA	2.2
1	C	274	ALA	2.2
1	C	268	ARG	2.2
1	A	172	GLU	2.2
1	E	223	ALA	2.2
1	F	228	SER	2.1
1	G	275	ALA	2.1
1	F	234	LEU	2.1
1	G	232	GLU	2.1
1	G	357	THR	2.1
1	F	265	ASN	2.1
1	A	231	ARG	2.1
1	C	230	ILE	2.1
1	G	311	LYS	2.1
1	C	295	LEU	2.1
1	C	320	ALA	2.1
1	B	204	PHE	2.1
1	G	282	GLY	2.1
1	C	267	MET	2.1
1	E	265	ASN	2.1
1	E	264	VAL	2.1
1	F	264	VAL	2.1
1	A	272	LYS	2.1
1	E	209	GLU	2.1
1	B	301	ILE	2.0
1	G	362	ARG	2.0
1	F	269	GLY	2.0
1	G	240	VAL	2.0
1	G	332	ILE	2.0
1	F	311	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

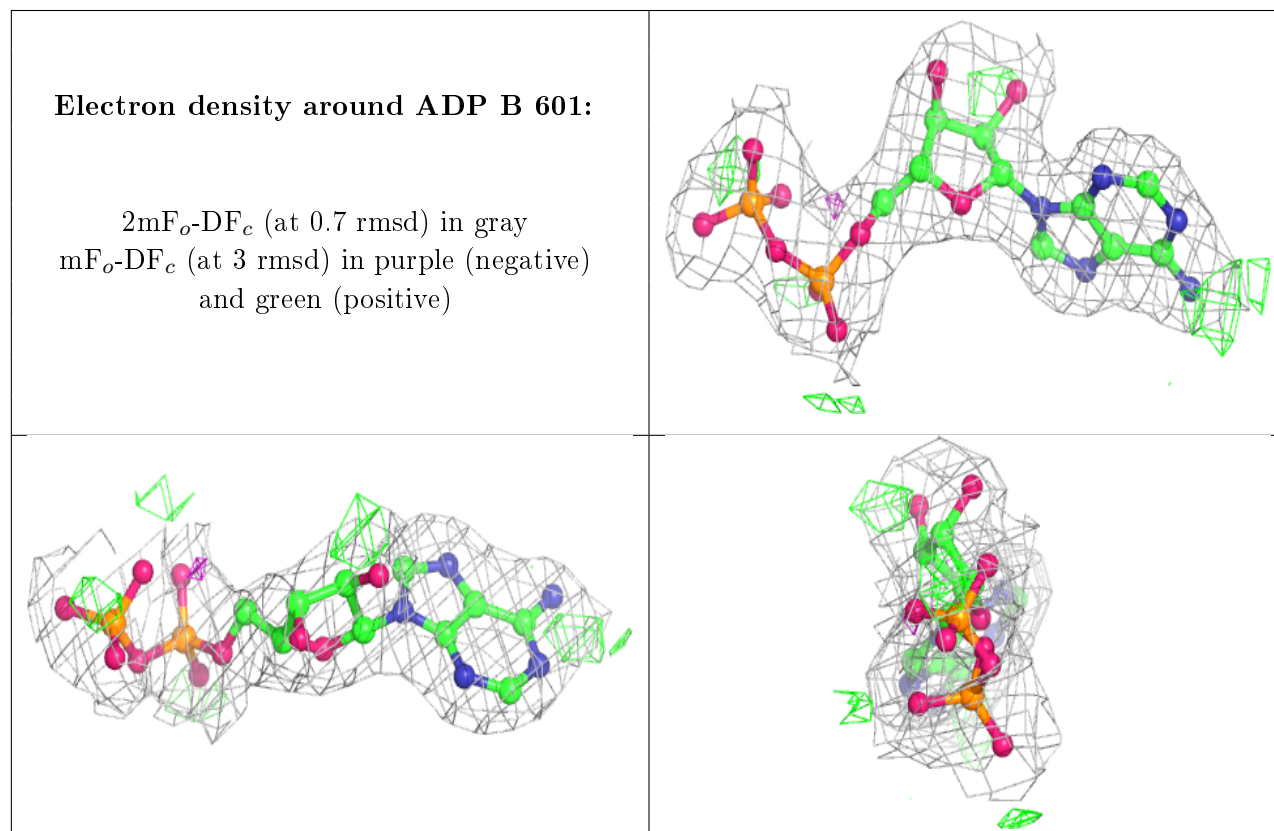
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	F	605	1/1	0.40	0.48	166,166,166,166	0
4	K	G	608	1/1	0.71	0.22	154,154,154,154	0
5	MPD	E	604	8/8	0.76	0.39	120,123,127,127	0
6	CA	E	607	1/1	0.78	0.20	126,126,126,126	0
5	MPD	B	608	8/8	0.80	0.28	93,98,109,118	0
5	MPD	D	605	8/8	0.80	0.36	108,112,116,116	0
5	MPD	A	604	8/8	0.80	0.20	106,109,115,123	0
5	MPD	G	604	8/8	0.80	0.37	78,99,109,117	0
6	CA	G	609	1/1	0.81	0.36	123,123,123,123	0
6	CA	G	607	1/1	0.82	0.20	114,114,114,114	0
5	MPD	D	606	8/8	0.85	0.28	79,99,108,113	0
5	MPD	G	605	8/8	0.85	0.32	114,117,141,153	0
6	CA	B	609	1/1	0.86	0.13	141,141,141,141	0
5	MPD	F	604	8/8	0.86	0.30	119,124,125,130	0
5	MPD	A	606	8/8	0.87	0.37	98,111,115,115	0
5	MPD	A	609	8/8	0.87	0.41	110,122,129,134	0
5	MPD	B	606	8/8	0.88	0.23	74,90,103,111	0
5	MPD	D	604	8/8	0.88	0.26	95,110,115,123	0
5	MPD	B	607	8/8	0.89	0.31	92,108,124,126	0
5	MPD	B	604	8/8	0.89	0.24	52,80,90,92	0
5	MPD	A	607	8/8	0.90	0.23	83,95,97,104	0
3	MG	B	602	1/1	0.90	0.18	29,29,29,29	0
5	MPD	A	608	8/8	0.90	0.38	103,110,120,123	0
5	MPD	C	604	8/8	0.90	0.31	102,107,112,117	0
6	CA	E	605	1/1	0.91	0.12	108,108,108,108	0
5	MPD	A	605	8/8	0.91	0.26	90,96,105,107	0
5	MPD	B	605	8/8	0.91	0.33	89,107,112,123	0
6	CA	A	611	1/1	0.93	0.38	107,107,107,107	0
6	CA	E	606	1/1	0.93	0.07	111,111,111,111	0
3	MG	A	602	1/1	0.94	0.15	33,33,33,33	0
6	CA	A	610	1/1	0.95	0.20	129,129,129,129	0
4	K	C	603	1/1	0.96	0.22	79,79,79,79	0
4	K	E	603	1/1	0.96	0.14	89,89,89,89	0
6	CA	F	606	1/1	0.97	0.11	110,110,110,110	0
3	MG	C	602	1/1	0.97	0.13	34,34,34,34	0
6	CA	G	606	1/1	0.97	0.21	88,88,88,88	0
2	ADP	B	601	27/27	0.97	0.19	30,48,62,127	0

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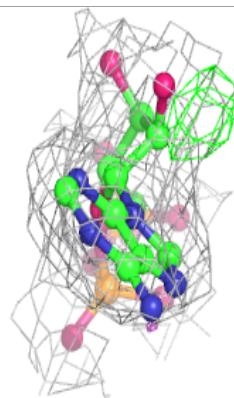
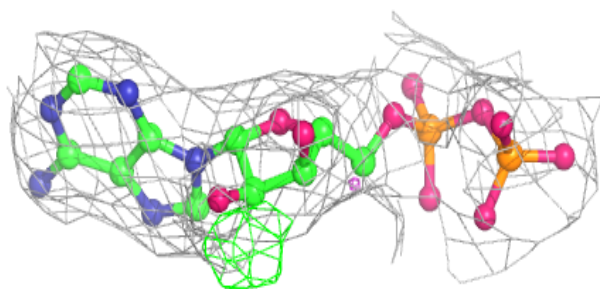
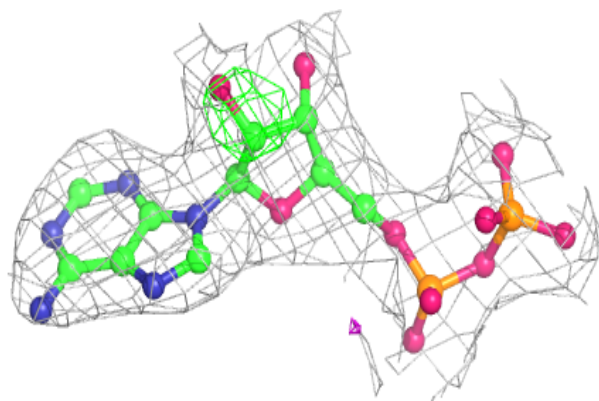
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	E	602	1/1	0.97	0.11	38,38,38,38	0
3	MG	F	602	1/1	0.97	0.11	28,28,28,28	0
6	CA	D	607	1/1	0.97	0.18	118,118,118,118	0
2	ADP	E	601	27/27	0.97	0.15	57,70,80,250	0
2	ADP	A	601	27/27	0.98	0.16	39,56,64,75	0
3	MG	G	602	1/1	0.98	0.14	25,25,25,25	0
2	ADP	G	601	27/27	0.98	0.17	41,50,65,94	0
2	ADP	C	601	27/27	0.98	0.17	43,55,64,66	0
4	K	B	603	1/1	0.98	0.22	62,62,62,62	0
2	ADP	D	601	27/27	0.98	0.17	36,57,70,80	0
4	K	D	603	1/1	0.98	0.16	64,64,64,64	0
2	ADP	F	601	27/27	0.98	0.19	38,62,74,86	0
3	MG	D	602	1/1	0.99	0.13	30,30,30,30	0
4	K	A	603	1/1	0.99	0.22	58,58,58,58	0
4	K	G	603	1/1	0.99	0.19	65,65,65,65	0
4	K	F	603	1/1	1.00	0.27	60,60,60,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

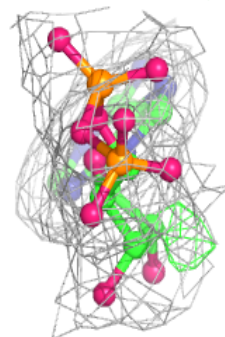
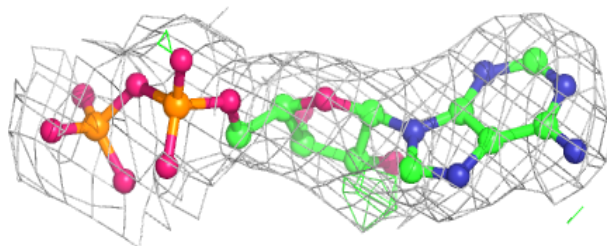
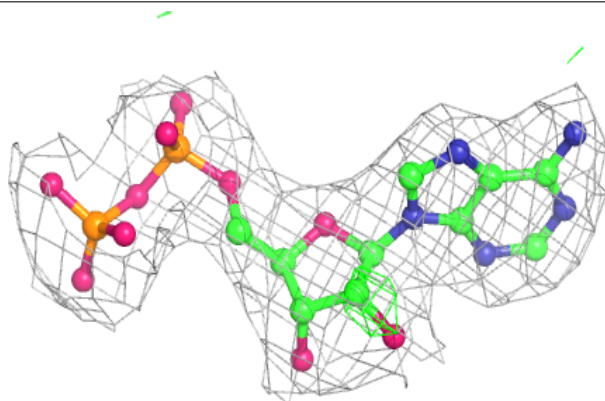


Electron density around ADP E 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

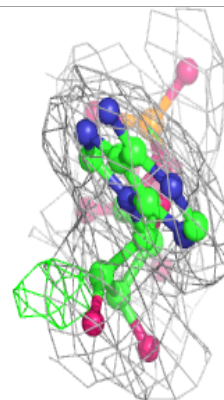
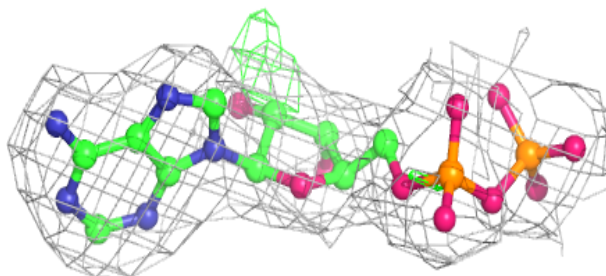
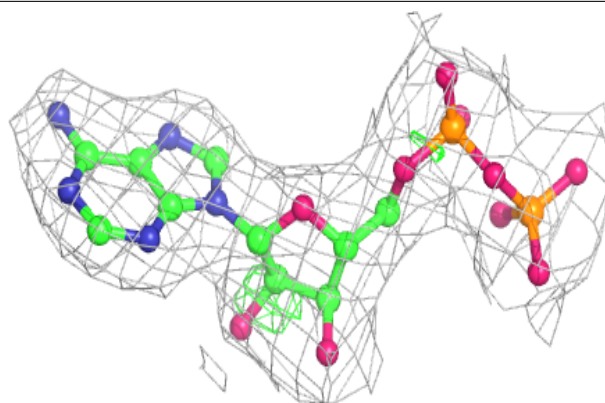
**Electron density around ADP A 601:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

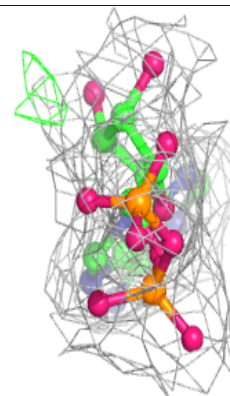
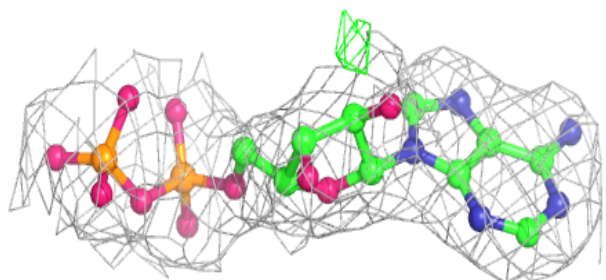
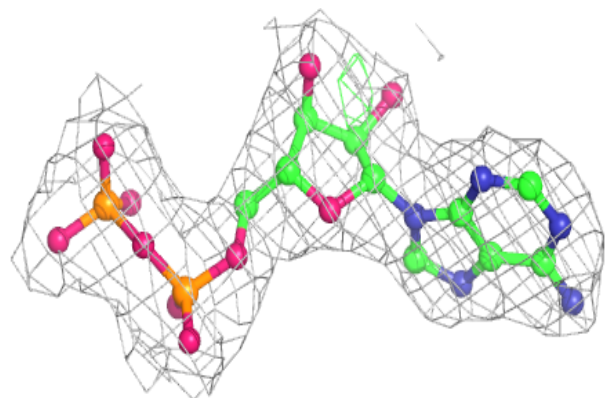


Electron density around ADP G 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

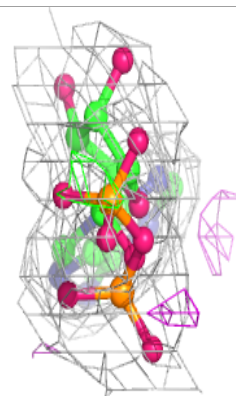
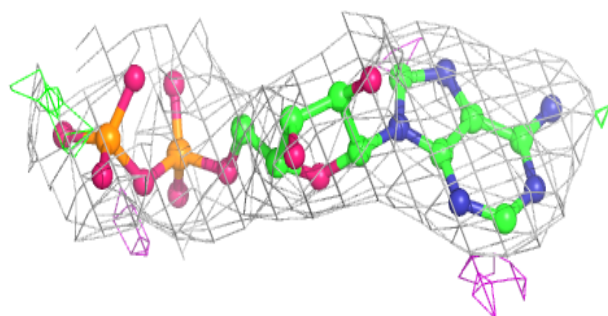
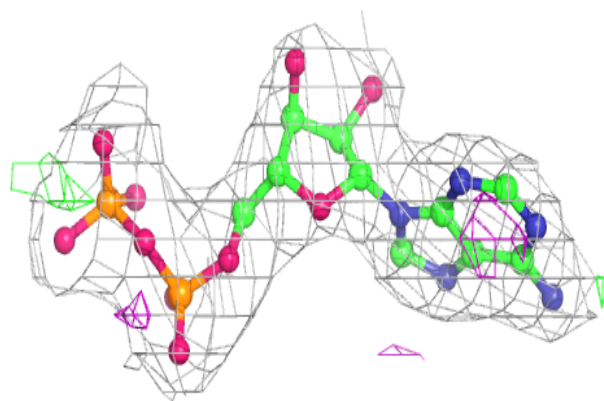
**Electron density around ADP C 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

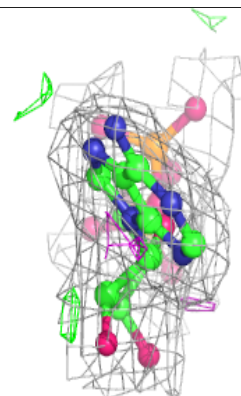
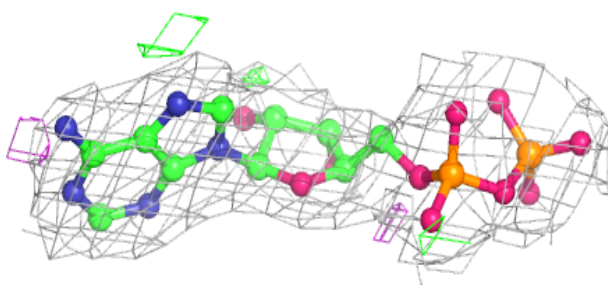
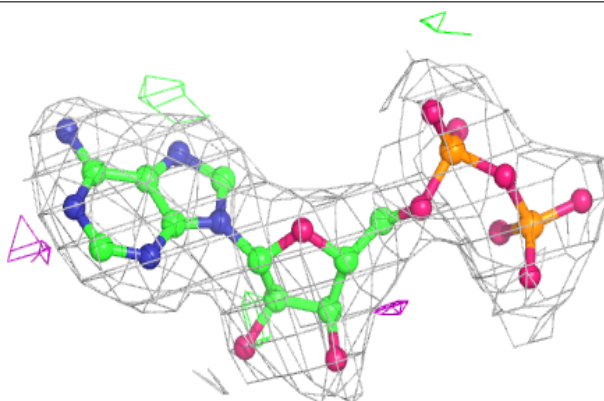


Electron density around ADP D 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP F 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.