



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:03 am GMT

PDB ID : 4A51  
Title : Crystal structure of human kinesin Eg5 in complex with 1-(3-(((2-Aminoethyl)thio)diphenylmethyl)phenyl)ethanone hydrochloride  
Authors : Kaan, H.Y.K.; Kozielski, F.  
Deposited on : 2011-10-24  
Resolution : 2.75 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

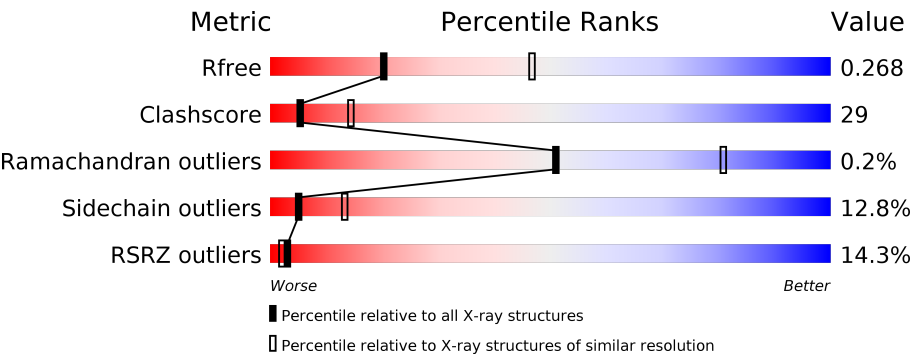
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.75 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 <sub>free</sub>	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	<div><div>11%</div><div><div></div><div>50%</div><div>33%</div><div>•</div><div>13%</div></div></div>
1	B	368	<div><div>12%</div><div><div></div><div>59%</div><div>24%</div><div>5%</div><div>12%</div></div></div>
1	C	368	<div><div>8%</div><div><div></div><div>55%</div><div>28%</div><div>5%</div><div>12%</div></div></div>
1	D	368	<div><div>7%</div><div><div></div><div>57%</div><div>29%</div><div>•</div><div>13%</div></div></div>
1	E	368	<div><div>14%</div><div><div></div><div>46%</div><div>36%</div><div>5%</div><div>13%</div></div></div>
1	F	368	<div><div>15%</div><div><div></div><div>36%</div><div>42%</div><div>10%</div><div>13%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	368	

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	DQ8	E	801	-	-	X	-

## 2 Entry composition [i](#)

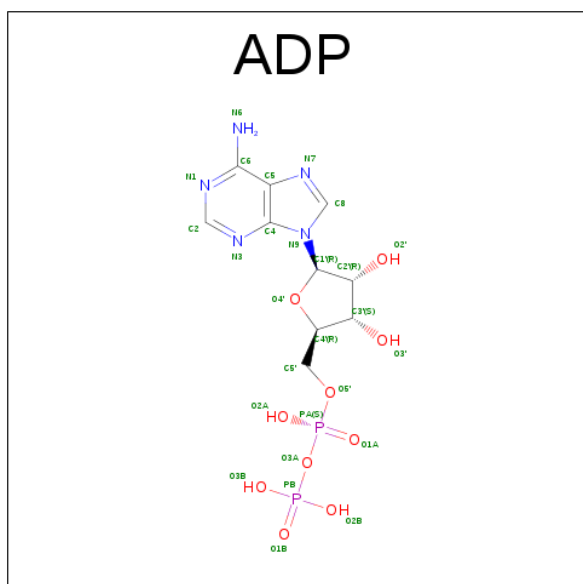
There are 7 unique types of molecules in this entry. The entry contains 18210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	1	0
			2522	1586	438	488	10			
1	B	324	Total	C	N	O	S	0	1	0
			2552	1602	446	494	10			
1	C	325	Total	C	N	O	S	0	1	0
			2551	1599	445	497	10			
1	D	322	Total	C	N	O	S	0	1	0
			2526	1585	438	493	10			
1	E	321	Total	C	N	O	S	0	0	0
			2504	1573	435	486	10			
1	F	319	Total	C	N	O	S	0	1	0
			2487	1559	433	486	9			
1	G	318	Total	C	N	O	S	0	0	0
			2446	1537	428	472	9			

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

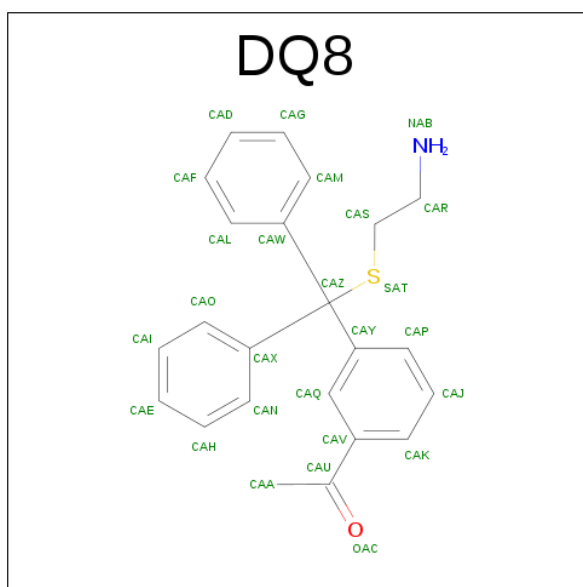


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G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

- Molecule 4 is 1-(3-{[(2-AMINOETHYL)SULFANYL](DIPHENYL)METHYL}PHENYL)ETHANONE (three-letter code: DQ8) (formula: C<sub>23</sub>H<sub>23</sub>NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	B	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	C	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	D	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	E	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	F	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	G	1	Total	C	N	O	S	0	0
			26	23	1	1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

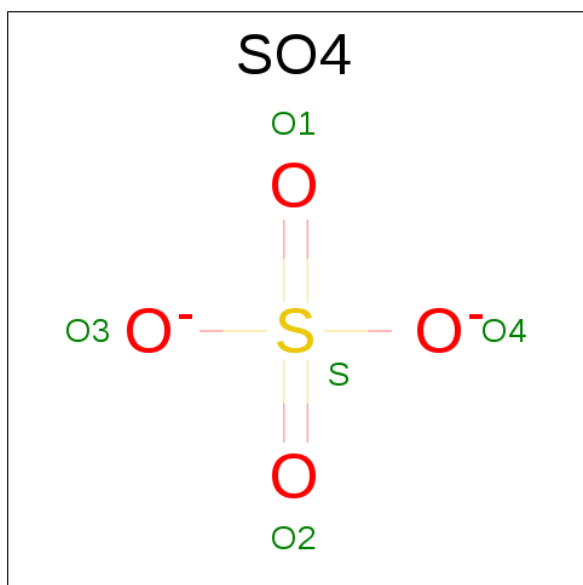
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cl	0	0
			1	1		
5	D	2	Total	Cl	0	0
			2	2		
5	E	1	Total	Cl	0	0
			1	1		
5	B	2	Total	Cl	0	0
			2	2		
5	C	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total	O	0	0
			32	32		
7	B	34	Total	O	0	0
			34	34		
7	C	47	Total	O	0	0
			47	47		
7	D	46	Total	O	0	0
			46	46		
7	E	22	Total	O	0	0
			22	22		
7	F	25	Total	O	0	0
			25	25		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	19	Total	O	0	0
			19	19		









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.84Å 156.40Å 170.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.75 29.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.99-2.75) 97.4 (29.99-2.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.221 , 0.280 0.212 , 0.268	Depositor DCC
$R_{free}$ test set	4936 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DQ8, SO4, ADP, CL

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	0.68	0/2563	0.83	0/3467
1	B	0.65	0/2593	0.80	1/3505 (0.0%)
1	C	0.66	0/2589	0.83	1/3503 (0.0%)
1	D	0.67	0/2566	0.80	1/3471 (0.0%)
1	E	0.53	0/2542	0.71	0/3440
1	F	0.54	0/2527	0.78	0/3421
1	G	0.52	0/2483	0.75	2/3364 (0.1%)
All	All	0.61	0/17863	0.79	5/24171 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ASN	N-CA-C	-6.89	92.40	111.00
1	G	57	LEU	CA-CB-CG	6.63	130.54	115.30
1	D	263	LEU	CA-CB-CG	-5.99	101.53	115.30
1	B	241	VAL	CB-CA-C	-5.68	100.60	111.40
1	G	57	LEU	N-CA-C	5.36	125.47	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	GLU	Peptide
1	C	189	ARG	Peptide
1	F	304	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2522	0	2550	138	0
1	B	2552	0	2584	78	0
1	C	2551	0	2563	117	0
1	D	2526	0	2539	88	0
1	E	2504	0	2520	139	0
1	F	2487	0	2494	222	0
1	G	2446	0	2442	232	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	4	0
2	D	27	0	12	5	0
2	E	27	0	12	5	0
2	F	27	0	12	3	0
2	G	27	0	12	2	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	26	0	23	7	0
4	B	26	0	23	8	0
4	C	26	0	23	2	0
4	D	26	0	23	4	0
4	E	26	0	23	9	0
4	F	26	0	23	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	26	0	23	7	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	D	5	0	0	0	0
7	A	32	0	0	2	0
7	B	34	0	0	0	0
7	C	47	0	0	2	0
7	D	46	0	0	2	0
7	E	22	0	0	1	0
7	F	25	0	0	1	0
7	G	19	0	0	0	0
All	All	18210	0	17937	1040	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (1040) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:TYR:CE2	1:E:86:VAL:HG21	1.82	1.12
1:F:89:ILE:HD12	1:F:101:ILE:HD11	1.23	1.12
1:A:141:HIS:O	1:A:207:LYS:NZ	1.83	1.11
1:F:136:ILE:HD13	1:F:263:LEU:HD12	1.29	1.09
1:F:171:LEU:HD12	1:F:220:LYS:HB3	1.34	1.09
1:E:215:GLU:HA	4:E:801:DQ8:HAH	1.31	1.08
1:C:206:ASN:ND2	1:C:208:ASP:HB2	1.69	1.06
1:G:181:ARG:HH11	1:G:181:ARG:HG2	1.15	1.05
2:F:601:ADP:H5'1	2:F:601:ADP:H8	1.19	1.05
2:D:601:ADP:H5'1	2:D:601:ADP:H8	1.19	1.05
1:E:92:GLU:OE1	1:E:92:GLU:N	1.88	1.04
1:F:86:VAL:HA	1:F:89:ILE:HD13	1.42	1.02
1:F:89:ILE:CD1	1:F:101:ILE:HD11	1.92	1.00
1:A:144:PHE:CD2	1:A:207:LYS:HD2	1.97	1.00
1:A:145:GLU:H	1:A:207:LYS:HZ3	1.03	0.99
1:D:31:ALA:O	1:D:34:LYS:HG3	1.62	0.98
1:A:192:ARG:NH1	1:A:322:ASP:OD1	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:TYR:CE1	1:G:86:VAL:HG21	1.98	0.98
1:D:255:LEU:HD12	1:D:256:VAL:H	1.26	0.97
1:A:144:PHE:HD2	1:A:207:LYS:HD2	1.28	0.97
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.46	0.96
1:E:306:THR:HG22	1:E:307:PRO:HD2	1.45	0.96
1:G:160:LEU:H	1:G:172:LEU:HD12	1.30	0.96
1:G:155:SER:OG	1:G:244:HIS:HB2	1.66	0.95
1:F:306:THR:HG22	1:F:307:PRO:HD2	1.50	0.94
1:C:306:THR:HG23	1:C:307:PRO:HD2	1.47	0.93
1:G:40:ILE:CD1	1:G:340:SER:HA	1.98	0.92
1:A:51:SER:HB2	1:A:65:THR:OG1	1.68	0.92
2:D:601:ADP:H5'1	2:D:601:ADP:C8	2.03	0.92
2:F:601:ADP:C8	2:F:601:ADP:H5'1	2.04	0.92
1:C:33:ARG:HD2	1:G:228:MET:HE1	1.50	0.91
1:A:306:THR:OG1	1:A:307:PRO:HD2	1.70	0.91
1:G:196:ILE:HD11	1:G:199:LEU:HB2	1.51	0.90
1:G:205:HIS:O	1:G:206:ASN:ND2	2.04	0.89
1:A:63:ARG:HH11	1:A:63:ARG:CG	1.86	0.89
1:A:264:VAL:HG21	1:A:320:LEU:HD11	1.56	0.87
1:D:102:PHE:CE1	1:D:320:LEU:HD13	2.09	0.87
1:G:56:GLY:C	1:G:58:ALA:HB3	1.92	0.87
1:G:181:ARG:HH11	1:G:181:ARG:CG	1.88	0.86
1:C:126:THR:HG23	1:C:129:GLU:HG2	1.57	0.86
1:B:162:GLU:OE1	1:B:231:TYR:OH	1.94	0.86
1:F:135:ILE:HG22	1:F:263:LEU:HD13	1.56	0.86
1:F:136:ILE:HD12	1:F:239:PHE:CD2	2.11	0.85
1:G:262:ASN:HD22	1:G:320:LEU:HD22	1.42	0.84
1:D:152:THR:OG1	1:D:246:LYS:O	1.95	0.84
1:E:215:GLU:CA	4:E:801:DQ8:HAH	2.08	0.84
1:F:215:GLU:HA	4:F:801:DQ8:HAH	1.58	0.84
1:F:94:ILE:HD11	1:F:147:LEU:HD21	1.60	0.84
1:E:82:TYR:CZ	1:E:86:VAL:HG21	2.13	0.83
1:F:230:ALA:HB3	1:F:234:ARG:HD2	1.61	0.83
1:F:82:TYR:O	1:F:86:VAL:HG13	1.78	0.83
1:F:172:LEU:HD23	1:F:216:LYS:HZ1	1.45	0.82
1:A:63:ARG:HH11	1:A:63:ARG:HG2	1.44	0.82
1:F:156:VAL:HG13	1:F:204:VAL:HG13	1.61	0.82
2:C:601:ADP:H5'1	2:C:601:ADP:H8	1.44	0.82
1:A:144:PHE:HE1	1:A:156:VAL:HG11	1.45	0.81
1:F:323:SER:O	1:F:330:THR:OG1	1.98	0.81
1:C:356:ALA:O	1:C:359:ILE:HG12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:HIS:HA	1:G:258:ILE:HG23	1.61	0.81
1:A:102:PHE:HB3	1:A:264:VAL:HB	1.60	0.81
1:F:158:VAL:HG21	1:F:213:ILE:HD11	1.63	0.81
1:C:206:ASN:HD22	1:C:208:ASP:HB2	1.45	0.81
1:D:87:CYS:HB2	1:D:88:PRO:HD3	1.63	0.80
1:F:136:ILE:HD13	1:F:263:LEU:CD1	2.11	0.80
1:D:299:ILE:HG23	1:D:359:ILE:HD11	1.63	0.80
1:F:158:VAL:HB	1:F:239:PHE:HE1	1.46	0.80
1:E:102:PHE:HB3	1:E:264:VAL:HB	1.62	0.80
1:F:170:ASP:HB2	1:F:182:LEU:HD11	1.64	0.80
1:B:160:LEU:HD13	1:B:239:PHE:HD2	1.46	0.80
1:E:300:THR:HG23	1:E:355:ARG:HH12	1.48	0.79
1:F:115:MET:O	1:F:136:ILE:HG12	1.81	0.79
1:F:322:ASP:O	1:F:328:THR:HG22	1.82	0.79
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.65	0.79
1:E:90:LEU:HD11	1:E:143:ILE:HD11	1.63	0.79
1:E:161:LEU:HD12	1:E:161:LEU:C	2.02	0.79
1:E:43:CYS:HB3	1:E:71:VAL:CG1	2.13	0.79
1:D:255:LEU:HD12	1:D:256:VAL:N	1.98	0.79
1:G:181:ARG:NH1	1:G:181:ARG:HG2	1.91	0.79
1:B:355:ARG:HB2	1:B:355:ARG:NH1	1.97	0.78
1:F:136:ILE:HB	1:F:137:PRO:HD3	1.63	0.78
1:G:82:TYR:CD1	1:G:86:VAL:HG21	2.18	0.78
1:F:86:VAL:HA	1:F:89:ILE:CD1	2.13	0.77
1:F:98:ASN:O	1:F:328:THR:OG1	1.99	0.77
1:G:262:ASN:HD22	1:G:320:LEU:CD2	1.97	0.77
1:E:306:THR:CG2	1:E:307:PRO:HD2	2.14	0.77
1:G:228:MET:HE2	1:G:228:MET:HA	1.64	0.77
1:G:347:LEU:HD12	1:G:348:SER:H	1.50	0.77
1:G:40:ILE:HD11	1:G:340:SER:HA	1.66	0.77
1:D:88:PRO:O	1:D:92:GLU:HG3	1.84	0.77
1:G:244:HIS:O	1:G:245:MET:HG3	1.85	0.77
1:E:86:VAL:CG2	1:E:87:CYS:N	2.48	0.77
1:G:156:VAL:HG12	1:G:204:VAL:O	1.85	0.76
1:G:312:ARG:O	1:G:313:GLU:HG2	1.84	0.76
1:C:119:ARG:HD3	1:C:211:TYR:OH	1.85	0.76
1:F:90:LEU:HD11	1:F:143:ILE:CD1	2.15	0.76
1:G:196:ILE:CD1	1:G:199:LEU:HB2	2.15	0.76
1:D:64:LYS:HE2	1:D:66:TYR:OH	1.86	0.76
1:F:49:GLU:HG2	1:F:67:THR:HG22	1.68	0.76
1:D:190:ASN:OD1	1:D:192:ARG:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:VAL:HG23	1:E:204:VAL:HB	1.68	0.75
1:G:311:TYR:CG	1:G:321:GLN:HG3	2.21	0.75
1:F:100:THR:HG22	1:F:262:ASN:HB2	1.66	0.75
1:E:218:ALA:O	1:E:222:THR:HG23	1.87	0.75
2:C:601:ADP:H5'1	2:C:601:ADP:C8	2.20	0.75
1:B:247:GLU:OE1	1:B:247:GLU:N	2.20	0.75
1:D:102:PHE:CZ	1:D:320:LEU:HD13	2.20	0.75
1:D:120:SER:HB3	1:D:121:PRO:HD2	1.67	0.75
1:F:270:GLU:HG2	1:F:271:ASN:OD1	1.86	0.75
1:G:184:MET:SD	1:G:194:VAL:HG11	2.27	0.75
1:G:41:VAL:CG1	1:G:338:PRO:HA	2.15	0.75
1:F:43:CYS:HB3	1:F:71:VAL:CG1	2.18	0.74
1:G:177:ASP:H	1:G:180:GLU:HG3	1.50	0.74
1:F:306:THR:CG2	1:F:307:PRO:HD2	2.17	0.74
1:B:178:VAL:HG13	1:B:220:LYS:HG2	1.69	0.74
1:G:90:LEU:HD11	1:G:143:ILE:HD11	1.70	0.74
1:A:66:TYR:HE2	1:A:351:GLU:OE1	1.70	0.74
1:B:355:ARG:HB2	1:B:355:ARG:HH11	1.52	0.74
1:C:207:LYS:NZ	1:G:123:GLU:HG2	2.03	0.74
1:F:323:SER:HA	1:F:328:THR:CG2	2.17	0.74
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.70	0.74
5:D:1363:CL:CL	7:D:2037:HOH:O	2.43	0.74
1:B:92:GLU:OE2	1:B:329:ARG:NH1	2.20	0.74
1:G:312:ARG:HG2	1:G:313:GLU:H	1.52	0.73
1:G:56:GLY:O	1:G:58:ALA:HB3	1.88	0.73
1:A:255:LEU:HD12	1:A:256:VAL:N	2.04	0.73
1:G:170:ASP:OD2	1:G:200:GLU:HB2	1.88	0.73
1:F:19:ILE:HG23	1:F:359:ILE:O	1.89	0.73
1:G:162:GLU:HG3	1:G:171:LEU:HD13	1.70	0.73
1:G:347:LEU:HD12	1:G:348:SER:N	2.04	0.73
1:A:152:THR:HG22	1:A:153:GLU:H	1.54	0.72
1:D:26:ARG:HH11	1:D:26:ARG:HG3	1.55	0.72
1:G:104:TYR:HB2	1:G:266:LEU:HD12	1.71	0.72
1:G:26:ARG:NH1	1:G:29:ASN:HD22	1.87	0.72
1:A:294:THR:HG22	1:A:317:THR:HG21	1.71	0.72
1:A:142:GLN:OE1	1:A:146:LYS:NZ	2.22	0.72
1:A:99:CYS:O	1:A:261:LEU:HD12	1.90	0.72
1:D:247:GLU:HG3	1:D:255:LEU:O	1.90	0.72
1:E:299:ILE:O	1:E:303:VAL:HG23	1.89	0.72
1:F:148:THR:O	1:F:151:GLY:N	2.21	0.71
1:G:270:GLU:HG2	1:G:271:ASN:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HD12	1:A:256:VAL:H	1.53	0.71
1:B:102:PHE:CE1	1:B:332:ILE:HG12	2.26	0.71
1:F:310:PRO:HB3	1:F:313:GLU:OE2	1.90	0.71
1:F:78:GLN:HG2	1:F:133:ALA:O	1.89	0.71
1:B:178:VAL:CG1	1:B:220:LYS:HG2	2.20	0.71
1:C:186:ASP:OD1	7:C:2030:HOH:O	2.08	0.71
1:G:270:GLU:N	1:G:270:GLU:OE1	2.22	0.71
1:C:186:ASP:OD2	1:C:312:ARG:NH2	2.23	0.71
1:A:144:PHE:CE1	1:A:156:VAL:HG11	2.25	0.71
1:D:54:THR:HG21	1:D:64:LYS:HG3	1.73	0.71
1:B:247:GLU:OE1	1:B:255:LEU:O	2.09	0.71
1:F:90:LEU:HD11	1:F:143:ILE:HD13	1.70	0.71
1:F:157:LYS:HG3	1:F:242:THR:HG23	1.73	0.71
1:C:126:THR:OG1	1:C:128:GLU:OE1	2.09	0.70
1:E:92:GLU:O	1:E:97:TYR:HB2	1.91	0.70
1:B:160:LEU:HD13	1:B:239:PHE:CD2	2.25	0.70
1:F:323:SER:HA	1:F:328:THR:HG23	1.72	0.70
2:D:601:ADP:H8	2:D:601:ADP:C5'	2.00	0.70
1:F:103:ALA:HB1	1:F:111:LYS:HG2	1.74	0.70
1:C:270:GLU:HG2	1:C:271:ASN:N	2.07	0.70
1:D:163:ILE:HG12	1:D:168:LEU:HD12	1.72	0.70
2:C:601:ADP:H8	2:C:601:ADP:C5'	2.04	0.70
1:F:90:LEU:O	1:F:93:VAL:HG13	1.92	0.69
1:B:18:ASN:N	1:B:18:ASN:OD1	2.25	0.69
1:E:139:THR:O	1:E:143:ILE:HG12	1.92	0.69
1:F:136:ILE:CD1	1:F:263:LEU:HD12	2.17	0.69
1:G:362:LYS:HB3	1:G:363:PRO:HD2	1.73	0.69
1:G:152:THR:OG1	1:G:153:GLU:N	2.24	0.69
1:E:82:TYR:HA	1:E:86:VAL:HG13	1.74	0.69
1:F:90:LEU:HD12	1:F:90:LEU:O	1.92	0.69
1:A:141:HIS:O	1:A:207:LYS:CE	2.40	0.69
1:F:98:ASN:OD1	1:F:260:LYS:HB3	1.92	0.69
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.74	0.69
1:E:170:ASP:CG	1:E:173:ASN:HB2	2.13	0.69
1:C:302:LEU:HB3	1:C:359:ILE:HG22	1.75	0.69
1:G:147:LEU:HD21	1:G:245:MET:HE1	1.73	0.69
1:G:192:ARG:O	1:G:321:GLN:NE2	2.25	0.68
1:A:59:ASP:C	1:A:59:ASP:OD1	2.30	0.68
1:D:247:GLU:OE1	1:D:255:LEU:HB3	1.93	0.68
1:E:161:LEU:HD12	1:E:161:LEU:O	1.93	0.68
1:F:244:HIS:CD2	1:F:258:ILE:HG22	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:PHE:CE2	1:F:207:LYS:N	2.62	0.68
1:C:361:ASN:O	1:C:363:PRO:HD3	1.93	0.68
1:F:82:TYR:HA	1:F:86:VAL:CG1	2.24	0.68
1:C:362:LYS:H	1:C:362:LYS:HD3	1.59	0.68
1:C:362:LYS:N	1:C:362:LYS:HD3	2.08	0.68
1:F:238:VAL:O	1:F:238:VAL:HG22	1.94	0.68
4:B:801:DQ8:HAO	4:B:801:DQ8:HAS2	1.75	0.67
2:E:601:ADP:H8	2:E:601:ADP:C5'	2.07	0.67
1:E:86:VAL:HG22	1:E:87:CYS:N	2.09	0.67
1:G:134:GLY:O	1:G:137:PRO:HD2	1.94	0.67
1:G:315:LYS:O	1:G:319:ILE:HD12	1.94	0.67
1:A:330:THR:HG22	1:A:331:SER:N	2.08	0.67
1:B:361:ASN:O	1:B:363:PRO:HD3	1.94	0.67
1:D:30:LEU:HD12	1:D:33:ARG:NH2	2.09	0.67
1:G:105:GLY:O	1:G:111:LYS:HE3	1.94	0.67
1:G:160:LEU:N	1:G:172:LEU:HD12	2.08	0.67
1:C:306:THR:CG2	1:C:307:PRO:HD2	2.20	0.67
1:F:141:HIS:C	1:F:141:HIS:HD1	1.97	0.67
1:G:161:LEU:HD12	1:G:161:LEU:C	2.15	0.67
1:G:295:LEU:O	1:G:298:VAL:HG12	1.95	0.67
1:G:111:LYS:NZ	2:G:601:ADP:O2B	2.28	0.67
1:E:147:LEU:HD21	1:E:245:MET:SD	2.34	0.67
1:E:82:TYR:CZ	1:E:86:VAL:CG2	2.78	0.67
1:G:111:LYS:HB2	1:G:111:LYS:NZ	2.10	0.67
1:A:62:SER:O	1:A:63:ARG:HG2	1.94	0.67
1:D:311:TYR:CD1	1:D:321:GLN:HG3	2.29	0.67
1:E:246:LYS:HA	1:E:256:VAL:HA	1.77	0.67
1:A:66:TYR:CE2	1:A:351:GLU:OE1	2.48	0.66
1:C:29:ASN:O	1:C:33:ARG:HG3	1.95	0.66
1:G:40:ILE:HG22	1:G:40:ILE:O	1.95	0.66
1:A:82:TYR:CD1	1:A:86:VAL:HB	2.30	0.66
1:C:54:THR:HG21	1:C:64:LYS:HG3	1.75	0.66
1:F:211:TYR:O	1:F:211:TYR:CD1	2.48	0.66
4:B:801:DQ8:CAO	4:B:801:DQ8:HAS2	2.26	0.66
1:B:157:LYS:NZ	1:B:201:GLU:OE1	2.18	0.66
1:G:298:VAL:HG23	1:G:310:PRO:HB3	1.77	0.66
1:C:360:LEU:HD12	1:C:360:LEU:H	1.61	0.66
1:E:298:VAL:HG22	1:E:309:VAL:HG12	1.78	0.66
1:E:82:TYR:O	1:E:86:VAL:HG13	1.95	0.66
1:A:327:ARG:O	1:A:363:PRO:HA	1.95	0.66
1:E:106:GLN:OE1	1:E:345:GLU:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:HA	1:A:244:HIS:O	1.96	0.65
1:E:28:PHE:CE1	1:E:338:PRO:HG2	2.31	0.65
1:F:162:GLU:OE2	1:F:237:SER:HB3	1.97	0.65
1:G:57:LEU:N	1:G:58:ALA:O	2.30	0.65
1:C:62:SER:O	1:C:63:ARG:HD2	1.95	0.65
1:F:102:PHE:HB3	1:F:264:VAL:CG1	2.26	0.65
1:C:19:ILE:CD1	1:C:359:ILE:HG13	2.25	0.65
1:F:124:GLU:HG2	1:F:125:TYR:CE1	2.31	0.65
1:B:102:PHE:HE1	1:B:332:ILE:CD1	2.09	0.65
1:G:209:GLU:O	1:G:213:ILE:HD13	1.97	0.65
1:A:98:ASN:O	1:A:328:THR:HG22	1.96	0.64
1:D:311:TYR:CG	1:D:321:GLN:HG3	2.32	0.64
2:E:601:ADP:C8	2:E:601:ADP:H5'1	2.32	0.64
1:D:196:ILE:HD11	1:D:319:ILE:HD11	1.80	0.64
2:E:601:ADP:H8	2:E:601:ADP:H5'1	1.62	0.64
1:F:86:VAL:O	1:F:89:ILE:HG12	1.97	0.64
1:G:317:THR:O	1:G:321:GLN:N	2.30	0.64
1:G:43:CYS:O	1:G:45:PRO:HD3	1.98	0.64
1:G:92:GLU:HG3	1:G:329:ARG:HD2	1.80	0.64
1:B:192:ARG:HB2	1:B:321:GLN:CD	2.17	0.64
1:F:136:ILE:HD12	1:F:239:PHE:HD2	1.62	0.64
1:F:68:PHE:HA	1:F:357:LYS:NZ	2.13	0.64
1:A:100:THR:OG1	1:A:323:SER:OG	2.10	0.64
1:E:43:CYS:HB3	1:E:71:VAL:HG11	1.80	0.64
1:A:306:THR:OG1	1:A:307:PRO:CD	2.46	0.64
1:B:69:ASP:O	1:B:70:MET:HG3	1.97	0.64
1:E:143:ILE:HD12	1:E:243:ILE:HD11	1.80	0.63
1:F:136:ILE:O	1:F:139:THR:HG22	1.97	0.63
1:F:162:GLU:HG3	1:F:171:LEU:CD2	2.28	0.63
1:F:82:TYR:CD2	1:F:86:VAL:HG11	2.33	0.63
1:G:161:LEU:HD12	1:G:162:GLU:N	2.13	0.63
1:G:270:GLU:HG2	1:G:271:ASN:N	2.11	0.63
1:B:87:CYS:HB2	1:B:88:PRO:HD3	1.80	0.63
1:F:161:LEU:HD12	1:F:161:LEU:C	2.19	0.63
1:F:102:PHE:HB3	1:F:264:VAL:HG12	1.79	0.63
4:E:801:DQ8:CAQ	4:E:801:DQ8:HAS1	2.28	0.63
1:E:86:VAL:HG22	1:E:87:CYS:H	1.61	0.63
1:C:178:VAL:HG13	1:C:220:LYS:HG3	1.81	0.63
1:F:82:TYR:CD2	1:F:138:ARG:HB2	2.34	0.63
1:D:306:THR:HG23	1:D:307:PRO:HD2	1.80	0.63
1:G:102:PHE:CE1	1:G:332:ILE:HG12	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:ARG:NH2	1:G:57:LEU:HA	2.13	0.63
1:F:28:PHE:CE1	1:F:338:PRO:HG2	2.34	0.63
4:F:801:DQ8:HAP	4:F:801:DQ8:CAL	2.28	0.63
1:A:178:VAL:CG1	1:A:220:LYS:HG2	2.29	0.63
1:G:228:MET:O	1:G:229:ASN:CG	2.36	0.63
1:E:143:ILE:HD12	1:E:243:ILE:CD1	2.29	0.62
1:G:82:TYR:CE1	1:G:86:VAL:CG2	2.80	0.62
1:C:262:ASN:O	1:C:263:LEU:HD23	1.99	0.62
4:C:801:DQ8:HAS1	4:C:801:DQ8:CAQ	2.30	0.62
1:D:190:ASN:OD1	1:D:191:LYS:N	2.32	0.62
1:E:156:VAL:HG12	1:E:243:ILE:HG12	1.79	0.62
1:B:352:TYR:HA	1:B:355:ARG:NH1	2.15	0.62
1:E:168:LEU:HD21	1:E:315:LYS:HD2	1.81	0.62
1:F:20:GLN:NE2	1:F:85:VAL:HG23	2.14	0.62
1:A:311:TYR:CD1	1:A:321:GLN:HG3	2.33	0.62
1:C:365:VAL:O	1:C:366:ASN:HB2	1.98	0.62
1:D:306:THR:CG2	1:D:307:PRO:HD2	2.30	0.62
1:E:120:SER:OG	1:E:132:LEU:HD23	1.99	0.62
1:E:154:PHE:CD1	1:E:154:PHE:O	2.52	0.62
1:E:82:TYR:HA	1:E:86:VAL:CG1	2.29	0.62
1:G:306:THR:HG22	1:G:307:PRO:HD2	1.80	0.62
1:A:178:VAL:HG13	1:A:220:LYS:CG	2.30	0.62
1:F:172:LEU:HD23	1:F:216:LYS:NZ	2.14	0.62
1:G:175:SER:O	1:G:176:SER:HB2	2.00	0.62
1:A:209:GLU:O	1:A:213:ILE:HG13	2.00	0.61
1:C:42:GLU:HA	1:C:42:GLU:OE1	2.00	0.61
1:F:306:THR:CB	1:F:307:PRO:HD2	2.28	0.61
1:C:206:ASN:N	1:C:206:ASN:OD1	2.33	0.61
1:F:158:VAL:HB	1:F:239:PHE:CE1	2.31	0.61
1:F:18:ASN:OD1	1:F:360:LEU:HB3	1.99	0.61
1:G:170:ASP:CG	1:G:173:ASN:HB2	2.21	0.61
1:A:145:GLU:N	1:A:207:LYS:HZ3	1.87	0.61
1:C:129:GLU:OE1	1:G:211:TYR:OH	2.16	0.61
1:E:270:GLU:O	1:E:271:ASN:HB2	1.99	0.61
1:E:54:THR:HG21	1:E:64:LYS:HD2	1.83	0.61
1:G:44:ASP:OD1	1:G:47:ARG:HB3	2.01	0.61
1:D:22:VAL:CG1	1:D:70:MET:HB2	2.30	0.61
1:G:21:VAL:CG1	1:G:357:LYS:HB3	2.30	0.61
1:C:27:PRO:HG2	1:G:227:LEU:HD21	1.81	0.61
1:D:143:ILE:HD13	1:D:243:ILE:HD11	1.81	0.61
1:E:309:VAL:HB	1:E:311:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HG12	1:A:263:LEU:HD12	1.83	0.61
1:F:184:MET:SD	1:F:318:ARG:HD3	2.41	0.61
2:D:601:ADP:C5'	2:D:601:ADP:C8	2.81	0.60
1:E:119:ARG:HD3	1:E:211:TYR:HE1	1.65	0.60
1:E:119:ARG:HG2	4:E:801:DQ8:HAO	1.82	0.60
1:F:204:VAL:HG21	1:F:210:VAL:HG23	1.83	0.60
1:A:308:HIS:ND1	7:A:2026:HOH:O	2.32	0.60
4:A:801:DQ8:CAQ	4:A:801:DQ8:HAS1	2.31	0.60
4:B:801:DQ8:CAS	4:B:801:DQ8:HAO	2.29	0.60
1:D:22:VAL:HG12	1:D:70:MET:HB2	1.83	0.60
1:A:189:ARG:O	1:A:190:ASN:HB2	2.01	0.60
1:E:90:LEU:HD11	1:E:143:ILE:CD1	2.30	0.60
1:F:29:ASN:OD1	1:F:32:GLU:HB2	2.02	0.60
1:G:53:ARG:HH21	1:G:57:LEU:HA	1.67	0.60
1:G:139:THR:O	1:G:143:ILE:HG12	2.01	0.60
1:B:130:ASP:OD1	1:B:131:PRO:HD2	2.01	0.60
1:C:25:CYS:O	1:C:74:ALA:HA	2.01	0.60
1:F:132:LEU:HD12	1:F:132:LEU:O	2.01	0.60
1:C:207:LYS:HZ1	1:G:123:GLU:HG2	1.66	0.60
1:G:362:LYS:CB	1:G:363:PRO:HD2	2.31	0.60
2:E:601:ADP:C5'	2:E:601:ADP:C8	2.84	0.60
1:F:100:THR:HG22	1:F:262:ASN:CB	2.31	0.60
1:E:328:THR:O	1:E:361:ASN:ND2	2.35	0.60
1:F:162:GLU:HG3	1:F:171:LEU:HD23	1.82	0.60
1:F:100:THR:CG2	1:F:262:ASN:HB2	2.32	0.60
1:E:40:ILE:HD12	1:E:343:LEU:HD13	1.84	0.60
1:E:82:TYR:CD2	1:E:86:VAL:HG21	2.35	0.60
1:F:43:CYS:HB3	1:F:71:VAL:HG12	1.82	0.60
1:G:196:ILE:HD11	1:G:199:LEU:CB	2.29	0.60
1:C:245:MET:HE3	1:C:257:LYS:HE3	1.84	0.60
1:E:136:ILE:HG12	1:E:263:LEU:HD12	1.84	0.60
1:F:18:ASN:HA	1:F:360:LEU:CB	2.31	0.60
1:G:196:ILE:CG1	1:G:199:LEU:HB2	2.32	0.60
1:G:47:ARG:O	1:G:47:ARG:HG3	2.00	0.59
1:C:293:LEU:HD21	1:C:297:ARG:NH2	2.17	0.59
1:G:26:ARG:NH1	1:G:29:ASN:ND2	2.49	0.59
1:E:92:GLU:H	1:E:92:GLU:CD	1.98	0.59
1:E:309:VAL:HG12	1:E:310:PRO:HD2	1.85	0.59
1:A:202:ILE:HG21	1:A:213:ILE:HD13	1.85	0.59
1:C:161:LEU:C	1:C:161:LEU:HD12	2.22	0.59
1:F:216:LYS:HZ3	1:F:217:GLY:N	1.98	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:GLN:O	1:G:81:VAL:HG23	2.02	0.59
1:A:141:HIS:C	1:A:141:HIS:ND1	2.55	0.59
1:B:89:ILE:HD13	1:B:101:ILE:HD11	1.85	0.59
1:E:120:SER:HB3	1:E:121:PRO:HD2	1.84	0.59
1:F:140:LEU:O	1:F:143:ILE:HG22	2.02	0.59
1:B:129:GLU:OE1	1:B:129:GLU:HA	2.03	0.59
1:B:154:PHE:HA	1:B:244:HIS:O	2.03	0.59
1:F:311:TYR:CD1	1:F:321:GLN:HG3	2.38	0.59
1:G:233:SER:OG	1:G:234:ARG:HD2	2.03	0.59
1:C:238:VAL:HG22	1:C:264:VAL:HG22	1.83	0.59
1:B:126:THR:HG23	1:B:129:GLU:HB2	1.84	0.59
1:C:75:SER:O	1:C:77:LYS:HD2	2.03	0.59
1:E:244:HIS:ND1	1:E:258:ILE:HG23	2.18	0.59
1:F:150:ASN:O	1:F:152:THR:HG23	2.03	0.59
1:G:314:SER:OG	1:G:317:THR:OG1	2.13	0.59
1:B:168:LEU:HD12	1:B:168:LEU:N	2.17	0.58
1:C:72:PHE:CD1	1:C:76:THR:HG21	2.38	0.58
1:F:128:GLU:O	1:F:129:GLU:OE2	2.21	0.58
1:G:296:GLY:O	1:G:300:THR:HG23	2.03	0.58
1:G:311:TYR:CD1	1:G:321:GLN:HG3	2.38	0.58
1:F:18:ASN:HA	1:F:360:LEU:HB3	1.84	0.58
1:B:111:LYS:HB2	1:B:111:LYS:NZ	2.19	0.58
1:F:141:HIS:C	1:F:141:HIS:ND1	2.56	0.58
1:G:116:GLU:HG2	4:G:801:DQ8:CAK	2.34	0.58
1:D:102:PHE:CE1	1:D:320:LEU:CD1	2.86	0.58
1:E:187:ASP:HB2	1:E:195:ILE:HG23	1.85	0.58
1:G:312:ARG:HG2	1:G:313:GLU:N	2.17	0.58
1:E:288:ILE:N	7:E:2015:HOH:O	2.36	0.58
1:C:118:GLU:OE1	1:G:226:THR:CG2	2.51	0.58
1:A:63:ARG:HH11	1:A:63:ARG:HG3	1.68	0.58
1:A:145:GLU:H	1:A:207:LYS:NZ	1.88	0.58
1:F:238:VAL:CG2	1:F:238:VAL:O	2.51	0.58
1:G:147:LEU:HD21	1:G:245:MET:CE	2.34	0.58
1:G:29:ASN:OD1	1:G:31:ALA:HB3	2.03	0.58
1:F:89:ILE:HG12	1:F:90:LEU:N	2.18	0.58
1:E:91:ASP:O	1:E:94:ILE:HB	2.04	0.57
1:F:102:PHE:CE1	1:F:332:ILE:HG12	2.39	0.57
1:E:154:PHE:HA	1:E:244:HIS:O	2.05	0.57
1:B:102:PHE:HE1	1:B:332:ILE:HD11	1.69	0.57
1:G:111:LYS:HB2	2:G:601:ADP:O2B	2.03	0.57
1:C:88:PRO:O	1:C:92:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:SER:OG	1:E:130:ASP:OD1	2.22	0.57
1:F:244:HIS:NE2	1:F:258:ILE:HG22	2.20	0.57
1:G:168:LEU:HD13	1:G:168:LEU:N	2.19	0.57
1:F:110:GLY:HA2	2:F:601:ADP:O2A	2.05	0.57
1:F:141:HIS:O	1:F:141:HIS:ND1	2.37	0.57
1:G:91:ASP:O	1:G:94:ILE:HG22	2.03	0.57
1:A:178:VAL:HG13	1:A:220:LYS:HG2	1.86	0.57
1:B:207:LYS:HD2	1:B:207:LYS:O	2.04	0.57
1:E:143:ILE:O	1:E:143:ILE:HG22	2.03	0.57
1:E:210:VAL:O	1:E:213:ILE:HG22	2.04	0.57
1:A:82:TYR:CE1	1:A:86:VAL:HB	2.39	0.57
1:E:103:ALA:HB1	1:E:111:LYS:CG	2.34	0.57
1:F:361:ASN:N	1:F:361:ASN:OD1	2.38	0.57
1:G:40:ILE:HD12	1:G:340:SER:HA	1.81	0.57
1:B:94:ILE:CD1	1:B:146:LYS:HE3	2.35	0.57
1:A:137:PRO:HG3	4:A:801:DQ8:HAP	1.87	0.57
1:B:20:GLN:OE1	1:B:70:MET:CE	2.53	0.57
1:B:288:ILE:HG13	1:B:289:ASN:N	2.20	0.57
1:C:327:ARG:HG2	1:C:362:LYS:O	2.05	0.57
1:F:158:VAL:HG21	1:F:213:ILE:CD1	2.35	0.57
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.04	0.56
1:D:130:ASP:OD1	1:D:131:PRO:HD2	2.05	0.56
4:F:801:DQ8:CAP	4:F:801:DQ8:CAL	2.78	0.56
1:C:126:THR:HG23	1:C:129:GLU:CG	2.30	0.56
1:C:207:LYS:HZ3	1:G:123:GLU:HG2	1.71	0.56
1:A:144:PHE:HB2	1:A:207:LYS:HZ2	1.70	0.56
1:G:82:TYR:CD1	1:G:86:VAL:CG2	2.88	0.56
1:G:107:THR:HB	1:G:270:GLU:OE2	2.05	0.56
1:A:230:ALA:HB3	1:A:234:ARG:NE	2.20	0.56
1:E:152:THR:HG22	1:E:153:GLU:H	1.70	0.56
1:F:190:ASN:OD1	1:F:191:LYS:N	2.38	0.56
1:G:155:SER:CB	1:G:244:HIS:HB2	2.35	0.56
1:G:44:ASP:OD1	1:G:46:VAL:HG23	2.06	0.56
1:A:330:THR:CG2	1:A:331:SER:N	2.69	0.56
1:A:33:ARG:HH11	1:A:33:ARG:HG2	1.71	0.56
1:D:247:GLU:OE2	1:D:257:LYS:HE3	2.05	0.56
1:D:92:GLU:O	1:D:97:TYR:HB2	2.06	0.56
1:F:19:ILE:HG21	1:F:359:ILE:HG22	1.87	0.56
1:G:170:ASP:OD1	1:G:170:ASP:C	2.43	0.56
1:G:21:VAL:HG11	1:G:357:LYS:HB3	1.87	0.56
1:E:299:ILE:HG23	1:E:359:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:GLN:O	1:G:20:GLN:HG3	2.05	0.56
1:D:26:ARG:NH2	1:D:32:GLU:OE2	2.36	0.56
1:F:139:THR:O	1:F:143:ILE:HB	2.05	0.56
1:G:186:ASP:N	1:G:186:ASP:OD1	2.39	0.56
1:G:136:ILE:HG12	1:G:263:LEU:HD13	1.88	0.56
1:A:127:TRP:CE2	1:A:128:GLU:HG3	2.40	0.56
1:C:288:ILE:H	1:C:288:ILE:HD12	1.72	0.56
1:F:144:PHE:HE2	1:F:207:LYS:N	2.02	0.56
1:A:69:ASP:O	1:A:70:MET:HG3	2.07	0.55
1:B:91:ASP:O	1:B:95:MET:HG2	2.07	0.55
1:D:18:ASN:N	1:D:361:ASN:H	2.04	0.55
1:D:186:ASP:OD2	1:D:312:ARG:NH2	2.39	0.55
1:G:295:LEU:O	1:G:299:ILE:HG12	2.06	0.55
1:E:323:SER:HA	1:E:328:THR:HB	1.88	0.55
1:E:87:CYS:SG	1:E:88:PRO:HD3	2.47	0.55
1:A:51:SER:HB2	1:A:65:THR:HG1	1.68	0.55
1:C:118:GLU:OE1	1:G:226:THR:HG21	2.07	0.55
4:D:801:DQ8:HAS1	4:D:801:DQ8:CAQ	2.36	0.55
1:E:161:LEU:CD1	1:E:161:LEU:C	2.72	0.55
1:G:158:VAL:HA	1:G:240:SER:O	2.07	0.55
1:A:289:ASN:O	1:A:293:LEU:HD13	2.07	0.55
1:D:34:LYS:HD2	1:D:35:ALA:N	2.22	0.55
1:G:312:ARG:CG	1:G:313:GLU:H	2.18	0.55
1:G:98:ASN:HD22	1:G:98:ASN:H	1.53	0.55
1:E:343:LEU:HD11	1:E:347:LEU:HD11	1.88	0.55
1:A:44:ASP:OD2	1:A:47:ARG:HD2	2.07	0.55
4:B:801:DQ8:HAS1	4:B:801:DQ8:CAQ	2.36	0.55
1:G:69:ASP:O	1:G:70:MET:HG2	2.07	0.55
1:E:310:PRO:HB2	1:E:313:GLU:HG3	1.87	0.55
1:F:230:ALA:CB	1:F:234:ARG:HD2	2.34	0.55
1:G:19:ILE:HG13	1:G:19:ILE:O	2.06	0.55
1:D:293:LEU:HD12	1:D:297:ARG:CZ	2.37	0.54
1:E:323:SER:O	1:E:330:THR:HG21	2.07	0.54
1:F:82:TYR:CE2	1:F:138:ARG:HB2	2.42	0.54
1:G:41:VAL:HG11	1:G:338:PRO:HA	1.86	0.54
1:C:89:ILE:O	1:C:93:VAL:HG23	2.07	0.54
1:D:26:ARG:NE	1:D:108:GLY:O	2.41	0.54
1:A:141:HIS:ND1	1:A:141:HIS:O	2.39	0.54
1:A:162:GLU:OE1	1:A:231:TYR:OH	2.04	0.54
1:F:135:ILE:O	1:F:139:THR:HB	2.08	0.54
1:F:19:ILE:HG22	1:F:360:LEU:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG13	1:B:220:LYS:CG	2.37	0.54
1:D:162:GLU:OE1	1:D:231:TYR:OH	2.13	0.54
1:F:325:GLY:HA2	1:F:360:LEU:O	2.07	0.54
1:A:132:LEU:N	1:A:132:LEU:HD23	2.21	0.54
1:A:288:ILE:HG23	1:A:289:ASN:H	1.71	0.54
1:D:90:LEU:HD22	1:D:139:THR:HG23	1.88	0.54
1:F:120:SER:OG	1:F:130:ASP:OD1	2.25	0.54
1:F:134:GLY:O	1:F:137:PRO:HD2	2.07	0.54
1:F:157:LYS:HB3	1:F:203:THR:HG22	1.89	0.54
1:F:44:ASP:OD1	1:F:47:ARG:HG3	2.08	0.54
1:G:136:ILE:HG12	1:G:263:LEU:CD1	2.37	0.54
1:G:362:LYS:HB3	1:G:363:PRO:CD	2.38	0.54
1:D:115:MET:O	1:D:136:ILE:HG13	2.07	0.54
1:F:114:THR:O	1:F:134:GLY:HA3	2.07	0.54
1:C:186:ASP:N	1:C:186:ASP:OD1	2.36	0.54
1:E:168:LEU:HB2	1:E:182:LEU:HB2	1.90	0.54
1:G:177:ASP:O	1:G:179:SER:N	2.41	0.54
1:G:361:ASN:C	1:G:362:LYS:HD2	2.29	0.54
1:G:137:PRO:HB3	4:G:801:DQ8:CAF	2.38	0.54
1:A:103:ALA:HB1	1:A:111:LYS:HB3	1.88	0.54
1:D:126:THR:HG23	1:D:129:GLU:HB2	1.90	0.54
1:F:143:ILE:HG12	1:F:243:ILE:HD11	1.88	0.54
1:F:185:PHE:O	1:F:194:VAL:HG12	2.08	0.54
1:F:91:ASP:O	1:F:94:ILE:HG22	2.08	0.54
1:E:170:ASP:HB2	1:E:182:LEU:HD11	1.90	0.53
1:G:215:GLU:HB2	4:G:801:DQ8:HAH	1.90	0.53
1:B:204:VAL:HG22	1:B:213:ILE:CD1	2.39	0.53
1:E:137:PRO:HD3	4:E:801:DQ8:HAJ	1.90	0.53
1:D:67:THR:O	1:D:357:LYS:HE2	2.08	0.53
1:F:54:THR:HG21	1:F:64:LYS:HG3	1.90	0.53
1:G:102:PHE:HB2	1:G:264:VAL:HG22	1.89	0.53
1:A:120:SER:OG	1:A:130:ASP:OD1	2.27	0.53
1:E:59:ASP:C	1:E:59:ASP:OD1	2.46	0.53
1:G:155:SER:HG	1:G:244:HIS:HB2	1.72	0.53
2:C:601:ADP:C5'	2:C:601:ADP:C8	2.85	0.53
1:F:100:THR:OG1	1:F:323:SER:OG	2.09	0.53
1:G:82:TYR:O	1:G:86:VAL:HG22	2.09	0.53
1:A:63:ARG:HG2	1:A:63:ARG:NH1	2.20	0.53
1:C:121:PRO:HG2	7:C:2023:HOH:O	2.07	0.53
1:D:26:ARG:HG3	1:D:26:ARG:NH1	2.22	0.53
1:E:352:TYR:O	1:E:355:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:VAL:CG1	1:G:204:VAL:O	2.56	0.53
1:G:144:PHE:CE2	1:G:206:ASN:C	2.82	0.53
1:A:130:ASP:OD1	1:A:131:PRO:HD2	2.08	0.53
1:B:206:ASN:OD1	1:B:208:ASP:HB2	2.09	0.53
1:C:150:ASN:OD1	1:C:152:THR:HG22	2.09	0.53
1:C:23:VAL:HG11	1:C:50:VAL:HG21	1.89	0.53
1:F:82:TYR:O	1:F:86:VAL:CG1	2.56	0.53
1:D:190:ASN:OD1	1:D:190:ASN:C	2.47	0.53
1:E:301:ALA:HB3	1:E:309:VAL:HG13	1.90	0.53
1:C:142:GLN:O	1:C:143:ILE:C	2.47	0.52
1:F:327:ARG:O	1:F:363:PRO:HA	2.09	0.52
1:F:163:ILE:HG12	1:F:168:LEU:HD23	1.91	0.52
1:G:56:GLY:O	1:G:57:LEU:HD13	2.09	0.52
1:D:102:PHE:HE1	1:D:320:LEU:HD13	1.70	0.52
1:E:125:TYR:N	1:E:125:TYR:CD1	2.78	0.52
1:G:40:ILE:HG22	1:G:52:VAL:HG13	1.91	0.52
1:B:184:MET:HE2	1:B:319:ILE:HG12	1.91	0.52
1:A:144:PHE:HB2	1:A:207:LYS:NZ	2.25	0.52
1:B:144:PHE:HZ	1:B:204:VAL:HG12	1.74	0.52
1:E:28:PHE:CD1	1:E:338:PRO:HG2	2.44	0.52
1:E:51:SER:OG	1:E:63:ARG:HD2	2.10	0.52
1:G:30:LEU:O	1:G:34:LYS:HE2	2.10	0.52
1:G:90:LEU:O	1:G:94:ILE:HB	2.09	0.52
1:A:63:ARG:CG	1:A:63:ARG:NH1	2.55	0.52
1:B:190:ASN:OD1	1:B:191:LYS:N	2.42	0.52
1:F:154:PHE:HD1	1:F:154:PHE:N	2.07	0.52
1:F:270:GLU:CG	1:F:271:ASN:OD1	2.57	0.52
1:B:94:ILE:HD12	1:B:146:LYS:HE3	1.91	0.52
1:F:221:ARG:O	1:F:224:ALA:N	2.42	0.52
1:C:365:VAL:O	1:C:366:ASN:CB	2.58	0.52
1:F:154:PHE:CD1	1:F:154:PHE:N	2.77	0.52
1:F:90:LEU:O	1:F:93:VAL:CG1	2.57	0.52
1:G:123:GLU:O	1:G:125:TYR:N	2.41	0.52
1:G:83:ARG:HA	1:G:87:CYS:SG	2.50	0.52
1:A:98:ASN:CB	1:A:328:THR:HG23	2.39	0.52
1:F:196:ILE:HB	1:F:199:LEU:HB2	1.91	0.52
1:G:166:GLU:HG3	1:G:315:LYS:CG	2.40	0.52
1:D:64:LYS:CE	1:D:66:TYR:OH	2.57	0.52
1:A:141:HIS:O	1:A:207:LYS:HE3	2.10	0.51
1:C:159:SER:HB2	1:C:199:LEU:HD11	1.92	0.51
4:B:801:DQ8:CAS	4:B:801:DQ8:CAO	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:354:HIS:CE1	1:G:358:ASN:HA	2.46	0.51
1:G:40:ILE:CD1	1:G:343:LEU:HB2	2.40	0.51
1:C:341:LEU:HD22	1:C:341:LEU:O	2.10	0.51
1:D:30:LEU:CD1	1:D:33:ARG:HH21	2.24	0.51
1:A:188:PRO:HD3	1:A:195:ILE:HD12	1.93	0.51
1:C:137:PRO:HD3	4:C:801:DQ8:HAJ	1.92	0.51
1:F:82:TYR:HA	1:F:86:VAL:HG12	1.93	0.51
1:A:109:THR:O	1:A:335:THR:CG2	2.59	0.51
1:E:86:VAL:HG23	1:E:87:CYS:N	2.24	0.51
1:G:244:HIS:C	1:G:245:MET:HG3	2.30	0.51
1:A:210:VAL:O	1:A:211:TYR:C	2.48	0.51
1:D:25:CYS:O	1:D:74:ALA:HA	2.10	0.51
1:F:89:ILE:HD12	1:F:101:ILE:CD1	2.16	0.51
1:A:23:VAL:HG21	1:A:68:PHE:CE2	2.46	0.51
1:E:103:ALA:CB	1:E:111:LYS:HG2	2.41	0.51
1:E:234:ARG:HD3	1:E:288:ILE:CG2	2.41	0.51
1:G:98:ASN:N	1:G:98:ASN:HD22	2.09	0.51
1:A:289:ASN:OD1	1:A:289:ASN:N	2.38	0.51
1:E:264:VAL:HG21	1:E:320:LEU:HD21	1.92	0.51
1:G:238:VAL:HG22	1:G:264:VAL:HB	1.92	0.51
1:E:29:ASN:ND2	1:E:32:GLU:OE1	2.42	0.51
4:A:801:DQ8:CAS	4:A:801:DQ8:CAQ	2.89	0.51
1:D:143:ILE:CD1	1:D:243:ILE:HD11	2.40	0.51
1:E:306:THR:HG22	1:E:307:PRO:CD	2.30	0.51
1:F:310:PRO:HB3	1:F:313:GLU:HG3	1.92	0.51
1:G:98:ASN:CB	1:G:260:LYS:HB3	2.41	0.50
1:G:41:VAL:HG13	1:G:338:PRO:HA	1.90	0.50
1:F:211:TYR:O	1:F:215:GLU:HB2	2.11	0.50
1:G:72:PHE:HB3	1:G:76:THR:OG1	2.12	0.50
1:G:124:GLU:HG2	1:G:125:TYR:CD2	2.46	0.50
1:C:365:VAL:HG12	1:C:366:ASN:N	2.24	0.50
1:D:26:ARG:HG3	1:D:27:PRO:O	2.11	0.50
1:E:127:TRP:CD1	1:E:211:TYR:HB2	2.46	0.50
1:E:126:THR:HG22	1:E:129:GLU:OE1	2.11	0.50
1:E:261:LEU:HD21	1:E:263:LEU:HD21	1.92	0.50
1:F:190:ASN:OD1	1:F:192:ARG:N	2.45	0.50
1:F:59:ASP:OD1	1:F:59:ASP:O	2.30	0.50
1:G:56:GLY:O	1:G:57:LEU:CD1	2.60	0.50
1:F:102:PHE:CB	1:F:264:VAL:HG13	2.42	0.50
1:F:119:ARG:HG2	4:F:801:DQ8:CAM	2.42	0.50
1:G:104:TYR:CD1	1:G:104:TYR:C	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ASP:C	1:C:265:ASP:OD1	2.50	0.50
1:G:181:ARG:CG	1:G:181:ARG:NH1	2.57	0.50
1:A:144:PHE:HD2	1:A:207:LYS:CD	2.12	0.50
1:C:102:PHE:HB3	1:C:264:VAL:HB	1.93	0.50
1:E:82:TYR:CA	1:E:86:VAL:HG13	2.42	0.50
1:F:320:LEU:O	1:F:323:SER:N	2.43	0.50
4:G:801:DQ8:CAO	4:G:801:DQ8:HAS2	2.42	0.50
1:E:234:ARG:HD3	1:E:288:ILE:HG21	1.92	0.49
1:F:265:ASP:C	1:F:265:ASP:OD1	2.50	0.49
1:C:19:ILE:HD13	1:C:359:ILE:HG13	1.91	0.49
1:D:212:GLN:CD	1:D:212:GLN:H	2.15	0.49
1:E:102:PHE:CB	1:E:264:VAL:HB	2.39	0.49
1:E:140:LEU:HD21	1:E:241:VAL:HG22	1.94	0.49
1:G:37:ALA:HB1	1:G:340:SER:OG	2.11	0.49
1:C:353:ALA:O	1:C:356:ALA:HB3	2.12	0.49
1:G:86:VAL:HG11	1:G:135:ILE:HG23	1.93	0.49
1:A:178:VAL:HG13	1:A:220:LYS:HG3	1.93	0.49
1:B:186:ASP:OD2	1:B:312:ARG:NH2	2.45	0.49
1:G:170:ASP:OD2	1:G:173:ASN:HB2	2.11	0.49
1:B:167:GLU:OE1	1:B:181:ARG:NE	2.43	0.49
1:F:154:PHE:H	1:F:154:PHE:HD1	1.61	0.49
1:G:123:GLU:C	1:G:125:TYR:H	2.13	0.49
1:A:187:ASP:OD1	1:A:188:PRO:HD2	2.12	0.49
1:B:205:HIS:N	1:B:209:GLU:OE1	2.32	0.49
1:E:29:ASN:ND2	1:E:32:GLU:HB2	2.28	0.49
1:G:111:LYS:HB2	1:G:111:LYS:HZ3	1.77	0.49
1:G:228:MET:CA	1:G:228:MET:HE2	2.38	0.49
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.95	0.49
1:F:215:GLU:CA	4:F:801:DQ8:HAH	2.36	0.49
1:G:111:LYS:HB2	1:G:111:LYS:HZ2	1.78	0.49
1:G:231:TYR:O	1:G:234:ARG:N	2.31	0.49
1:A:271:ASN:O	7:A:2025:HOH:O	2.20	0.49
1:C:162:GLU:OE1	1:C:231:TYR:OH	2.29	0.49
1:C:309:VAL:HB	1:C:311:TYR:CE2	2.48	0.49
1:G:295:LEU:O	1:G:295:LEU:HD12	2.12	0.49
1:G:354:HIS:CE1	1:G:358:ASN:OD1	2.66	0.49
1:A:40:ILE:HD13	1:A:343:LEU:HB2	1.95	0.48
1:D:161:LEU:HD12	1:D:161:LEU:C	2.34	0.48
1:F:173:ASN:OD1	1:F:174:PRO:HD2	2.13	0.48
1:G:160:LEU:H	1:G:172:LEU:CD1	2.13	0.48
1:G:26:ARG:HD2	1:G:27:PRO:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:TYR:CB	1:G:321:GLN:HG3	2.43	0.48
1:D:119:ARG:HA	1:D:130:ASP:OD2	2.12	0.48
1:G:295:LEU:HD12	1:G:298:VAL:HG12	1.95	0.48
1:C:262:ASN:C	1:C:263:LEU:HD23	2.32	0.48
1:E:170:ASP:OD2	1:E:173:ASN:HB2	2.13	0.48
1:F:309:VAL:HG13	1:F:311:TYR:CE2	2.47	0.48
1:F:40:ILE:HD13	1:F:340:SER:HA	1.94	0.48
1:G:167:GLU:HB2	1:G:169:PHE:CE1	2.48	0.48
1:B:291:SER:HA	1:B:314:SER:HB2	1.95	0.48
1:C:143:ILE:HD13	1:C:243:ILE:HD11	1.94	0.48
1:E:134:GLY:O	1:E:137:PRO:HD2	2.13	0.48
1:E:82:TYR:CD2	1:E:86:VAL:HG11	2.48	0.48
1:F:264:VAL:HG11	1:F:320:LEU:HD21	1.95	0.48
1:F:311:TYR:CE1	1:F:321:GLN:HG3	2.48	0.48
1:G:137:PRO:HB3	4:G:801:DQ8:HAF	1.94	0.48
1:D:139:THR:HG21	1:D:261:LEU:HD23	1.94	0.48
1:F:136:ILE:HG23	1:F:239:PHE:CE2	2.49	0.48
1:G:361:ASN:O	1:G:362:LYS:HD2	2.13	0.48
1:A:123:GLU:O	1:A:125:TYR:N	2.46	0.48
1:A:119:ARG:HD3	4:A:801:DQ8:CAG	2.44	0.48
1:E:163:ILE:HG12	1:E:168:LEU:CD1	2.43	0.48
1:A:178:VAL:CG1	1:A:220:LYS:CG	2.90	0.48
1:C:308:HIS:ND1	1:C:308:HIS:O	2.46	0.48
1:C:77:LYS:HG2	1:G:219:ALA:HB1	1.94	0.48
1:F:239:PHE:C	1:F:239:PHE:CD1	2.86	0.48
1:G:102:PHE:CB	1:G:264:VAL:HG22	2.43	0.48
1:D:171:LEU:HD13	1:D:221:ARG:HB2	1.96	0.48
1:E:25:CYS:HB2	1:E:336:ILE:CG1	2.43	0.48
1:G:311:TYR:HB2	1:G:321:GLN:HG3	1.96	0.48
1:E:90:LEU:O	1:E:90:LEU:HD12	2.14	0.48
1:F:68:PHE:HA	1:F:357:LYS:HZ2	1.78	0.48
1:F:49:GLU:HG2	1:F:67:THR:CG2	2.42	0.48
1:C:33:ARG:CD	1:G:228:MET:HE1	2.33	0.48
1:G:40:ILE:CG2	1:G:40:ILE:O	2.61	0.48
1:B:29:ASN:OD1	1:B:31:ALA:HB3	2.14	0.48
1:C:293:LEU:HD21	1:C:297:ARG:HH22	1.78	0.48
1:G:147:LEU:HD11	1:G:245:MET:CE	2.44	0.48
1:G:298:VAL:O	1:G:302:LEU:HD12	2.14	0.48
1:A:158:VAL:HG12	1:A:241:VAL:HG22	1.96	0.47
1:C:360:LEU:HD12	1:C:360:LEU:N	2.27	0.47
1:F:140:LEU:O	1:F:143:ILE:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:ASP:OD1	1:G:172:LEU:N	2.47	0.47
1:G:158:VAL:HG22	1:G:239:PHE:CE1	2.48	0.47
1:A:288:ILE:HG23	1:A:289:ASN:OD1	2.14	0.47
1:B:102:PHE:CD1	1:B:332:ILE:HG12	2.49	0.47
1:C:144:PHE:O	1:C:146:LYS:N	2.48	0.47
1:E:49:GLU:HG2	1:E:67:THR:CG2	2.44	0.47
1:G:102:PHE:HB2	1:G:264:VAL:O	2.14	0.47
1:G:26:ARG:HH12	1:G:29:ASN:ND2	2.11	0.47
1:G:35:ALA:CB	1:G:341:LEU:HD11	2.45	0.47
1:C:320:LEU:O	1:C:323:SER:HB2	2.14	0.47
1:E:323:SER:HB3	1:E:330:THR:HG21	1.94	0.47
1:C:135:ILE:HG22	1:C:263:LEU:HD13	1.95	0.47
1:E:245:MET:O	1:E:257:LYS:N	2.44	0.47
1:E:300:THR:CG2	1:E:355:ARG:HH12	2.21	0.47
1:F:161:LEU:HD12	1:F:161:LEU:O	2.14	0.47
1:F:345:GLU:HA	1:F:345:GLU:OE1	2.14	0.47
1:F:19:ILE:CG2	1:F:359:ILE:O	2.62	0.47
1:B:162:GLU:OE2	1:B:221:ARG:NE	2.46	0.47
1:D:196:ILE:CD1	1:D:319:ILE:HD11	2.44	0.47
1:E:103:ALA:HB1	1:E:111:LYS:HG2	1.97	0.47
1:G:77:LYS:O	1:G:80:ASP:HB2	2.14	0.47
1:B:192:ARG:HD2	1:B:322:ASP:OD1	2.15	0.47
1:D:142:GLN:O	1:D:146:LYS:HB2	2.15	0.47
1:D:90:LEU:O	1:D:90:LEU:HD12	2.14	0.47
1:F:128:GLU:HA	1:F:128:GLU:OE1	2.13	0.47
1:F:156:VAL:CG1	1:F:204:VAL:HG13	2.38	0.47
1:F:301:ALA:O	1:F:305:ARG:HA	2.14	0.47
1:G:98:ASN:HB3	1:G:260:LYS:HB3	1.95	0.47
1:G:311:TYR:CG	1:G:321:GLN:CG	2.97	0.47
1:A:98:ASN:HB2	1:A:328:THR:HG23	1.96	0.47
1:C:178:VAL:CG1	1:C:220:LYS:HG3	2.43	0.47
1:D:163:ILE:HG12	1:D:168:LEU:CD1	2.42	0.47
2:E:601:ADP:H8	2:E:601:ADP:H5'2	1.79	0.47
1:F:135:ILE:CG2	1:F:263:LEU:HD13	2.38	0.47
1:B:144:PHE:CZ	1:B:204:VAL:HG12	2.50	0.47
1:F:271:ASN:O	7:F:2020:HOH:O	2.20	0.47
1:G:166:GLU:HG3	1:G:315:LYS:HG2	1.95	0.47
1:G:262:ASN:ND2	1:G:320:LEU:CD2	2.74	0.47
1:A:123:GLU:C	1:A:125:TYR:H	2.19	0.47
1:C:309:VAL:O	1:C:311:TYR:N	2.45	0.47
1:E:128:GLU:HG2	1:E:141:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:THR:CG2	1:E:153:GLU:H	2.26	0.47
1:B:40:ILE:HD13	1:B:340:SER:HA	1.97	0.47
1:C:161:LEU:O	1:C:161:LEU:HD12	2.13	0.47
1:C:264:VAL:HG21	1:C:320:LEU:HD21	1.97	0.47
1:E:86:VAL:O	1:E:90:LEU:N	2.46	0.47
1:G:308:HIS:O	1:G:310:PRO:O	2.32	0.47
1:G:343:LEU:O	1:G:347:LEU:HG	2.14	0.47
1:G:53:ARG:NH2	1:G:57:LEU:CA	2.78	0.47
1:D:162:GLU:OE1	1:D:231:TYR:CE2	2.68	0.46
1:E:173:ASN:CG	1:E:174:PRO:HD2	2.35	0.46
1:E:89:ILE:O	1:E:93:VAL:HG23	2.15	0.46
1:F:101:ILE:HA	1:F:331:SER:O	2.14	0.46
1:F:68:PHE:HA	1:F:357:LYS:CE	2.44	0.46
1:D:197:LYS:NZ	1:F:58:ALA:O	2.45	0.46
1:G:20:GLN:HB2	1:G:69:ASP:OD2	2.15	0.46
1:C:72:PHE:HB3	1:C:76:THR:HG21	1.97	0.46
1:F:317:THR:O	1:F:321:GLN:N	2.48	0.46
1:G:293:LEU:HA	1:G:352:TYR:HE2	1.80	0.46
4:G:801:DQ8:HAA1	4:G:801:DQ8:HAK	1.61	0.46
1:C:128:GLU:OE2	1:C:207:LYS:HE3	2.15	0.46
1:E:178:VAL:HG22	1:E:178:VAL:O	2.16	0.46
1:G:123:GLU:HA	1:G:123:GLU:OE1	2.15	0.46
1:A:156:VAL:O	1:A:156:VAL:HG13	2.15	0.46
1:E:152:THR:HG22	1:E:153:GLU:N	2.29	0.46
1:E:158:VAL:HA	1:E:240:SER:O	2.15	0.46
1:F:102:PHE:HD1	1:F:102:PHE:O	1.97	0.46
1:F:89:ILE:HG12	1:F:90:LEU:H	1.80	0.46
1:A:30:LEU:CD2	1:A:33:ARG:HD2	2.46	0.46
1:F:293:LEU:CD2	1:F:297:ARG:HH21	2.29	0.46
1:F:59:ASP:C	1:F:59:ASP:OD1	2.53	0.46
1:G:177:ASP:N	1:G:180:GLU:HG3	2.26	0.46
1:G:136:ILE:CG1	1:G:263:LEU:HD13	2.46	0.46
1:G:347:LEU:O	1:G:351:GLU:N	2.44	0.46
1:A:293:LEU:H	1:A:293:LEU:CD1	2.29	0.46
1:B:139:THR:O	1:B:143:ILE:HG13	2.15	0.46
1:E:103:ALA:HB1	1:E:111:LYS:HG3	1.97	0.46
1:F:91:ASP:OD1	1:F:146:LYS:NZ	2.48	0.46
1:A:19:ILE:HG22	1:A:361:ASN:OD1	2.15	0.46
1:E:142:GLN:O	1:E:146:LYS:HB2	2.15	0.46
1:A:104:TYR:CE2	1:A:352:TYR:CE1	3.04	0.46
1:C:306:THR:CG2	1:C:307:PRO:CD	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:801:DQ8:CAL	4:D:801:DQ8:CAP	2.94	0.46
1:E:154:PHE:CD1	1:E:154:PHE:C	2.89	0.46
1:F:299:ILE:HA	1:F:359:ILE:HD11	1.98	0.46
1:F:94:ILE:HD11	1:F:147:LEU:CD2	2.38	0.46
1:C:149:ASP:OD1	1:C:149:ASP:N	2.50	0.45
1:C:308:HIS:CG	1:C:308:HIS:O	2.68	0.45
1:C:327:ARG:HB3	1:C:363:PRO:HA	1.98	0.45
1:D:30:LEU:CD1	1:D:33:ARG:NH2	2.76	0.45
1:G:40:ILE:HD12	1:G:343:LEU:HB2	1.99	0.45
1:D:40:ILE:O	1:D:52:VAL:HA	2.15	0.45
4:E:801:DQ8:HAN	4:E:801:DQ8:CAQ	2.46	0.45
1:F:28:PHE:CD1	1:F:338:PRO:HG2	2.50	0.45
1:G:293:LEU:CD2	1:G:297:ARG:HE	2.30	0.45
1:G:26:ARG:CZ	1:G:29:ASN:HD22	2.28	0.45
1:B:79:ILE:O	1:B:83:ARG:HB2	2.17	0.45
1:E:289:ASN:O	1:E:293:LEU:HB2	2.17	0.45
1:F:49:GLU:CG	1:F:67:THR:HG22	2.44	0.45
1:G:40:ILE:HD11	1:G:340:SER:CA	2.42	0.45
1:A:40:ILE:HD12	1:A:52:VAL:CG1	2.47	0.45
1:C:92:GLU:O	1:C:97:TYR:HB2	2.17	0.45
1:D:120:SER:HB3	1:D:121:PRO:CD	2.40	0.45
1:F:293:LEU:HD22	1:F:297:ARG:HH21	1.79	0.45
1:A:144:PHE:CB	1:A:207:LYS:HZ2	2.29	0.45
4:A:801:DQ8:HAP	4:A:801:DQ8:CAL	2.46	0.45
1:B:130:ASP:OD1	1:B:131:PRO:CD	2.64	0.45
1:B:106:GLN:NE2	1:B:345:GLU:HG3	2.32	0.45
1:C:163:ILE:HG12	1:C:168:LEU:HD23	1.97	0.45
1:D:18:ASN:HB2	1:D:360:LEU:HD23	1.98	0.45
1:G:190:ASN:O	1:G:192:ARG:N	2.50	0.45
1:G:73:GLY:O	1:G:75:SER:N	2.49	0.45
1:C:146:LYS:HE2	1:C:146:LYS:HB2	1.70	0.45
1:C:173:ASN:ND2	1:E:57:LEU:HD22	2.32	0.45
1:C:187:ASP:HA	1:C:188:PRO:HD3	1.88	0.45
1:G:132:LEU:HD23	1:G:132:LEU:HA	1.87	0.45
1:G:309:VAL:N	1:G:310:PRO:HD2	2.32	0.45
1:D:322:ASP:OD1	1:D:322:ASP:N	2.47	0.45
1:G:196:ILE:HD12	1:G:196:ILE:C	2.37	0.45
1:G:308:HIS:C	1:G:310:PRO:HD2	2.37	0.45
1:F:123:GLU:C	1:F:123:GLU:CD	2.75	0.45
1:F:205:HIS:O	1:F:206:ASN:HB3	2.17	0.45
1:F:25:CYS:O	1:F:74:ALA:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:TYR:CE2	1:F:86:VAL:HG21	2.51	0.45
1:G:310:PRO:HB2	1:G:311:TYR:CD1	2.52	0.45
1:G:87:CYS:HB2	1:G:88:PRO:HD3	1.98	0.45
1:A:78:GLN:NE2	1:A:113:PHE:CE1	2.85	0.45
1:B:162:GLU:CD	1:B:171:LEU:HD11	2.36	0.45
1:B:82:TYR:CD1	1:B:86:VAL:HB	2.51	0.45
1:D:140:LEU:HA	1:D:140:LEU:HD23	1.75	0.45
1:E:294:THR:O	1:E:295:LEU:C	2.54	0.45
1:F:144:PHE:O	1:F:147:LEU:N	2.50	0.45
1:A:136:ILE:HG13	1:A:263:LEU:HD13	1.99	0.45
1:A:98:ASN:C	1:A:328:THR:HG22	2.36	0.45
1:A:106:GLN:NE2	1:A:345:GLU:HG2	2.32	0.45
1:B:92:GLU:O	1:B:97:TYR:HB2	2.17	0.45
1:D:18:ASN:HA	1:D:360:LEU:HA	1.98	0.45
1:G:302:LEU:CD1	1:G:324:LEU:HD23	2.47	0.45
1:B:149:ASP:OD1	1:B:149:ASP:N	2.50	0.44
4:E:801:DQ8:CAL	4:E:801:DQ8:CAP	2.92	0.44
1:A:202:ILE:HG21	1:A:213:ILE:CD1	2.46	0.44
1:B:152:THR:HA	1:B:246:LYS:O	2.17	0.44
1:F:118:GLU:O	4:F:801:DQ8:HAG	2.17	0.44
1:F:308:HIS:CG	1:F:308:HIS:O	2.68	0.44
1:A:123:GLU:HB2	1:A:124:GLU:H	1.44	0.44
1:A:288:ILE:HG13	1:A:289:ASN:N	2.32	0.44
4:A:801:DQ8:CAS	4:A:801:DQ8:HAQ	2.48	0.44
1:C:39:SER:HA	1:C:338:PRO:O	2.17	0.44
1:F:23:VAL:HA	1:F:334:ALA:O	2.18	0.44
1:G:299:ILE:HG12	1:G:299:ILE:H	1.61	0.44
1:A:152:THR:HG22	1:A:153:GLU:N	2.29	0.44
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.32	0.44
1:E:239:PHE:C	1:E:239:PHE:CD1	2.91	0.44
1:C:190:ASN:OD1	1:C:190:ASN:C	2.55	0.44
1:C:266:LEU:HD22	1:C:316:LEU:HD21	1.99	0.44
1:F:241:VAL:HG12	1:F:261:LEU:HB3	1.99	0.44
1:G:20:GLN:CG	1:G:20:GLN:O	2.64	0.44
1:A:192:ARG:HH21	1:A:327:ARG:NH1	2.15	0.44
1:A:90:LEU:O	1:A:93:VAL:HG22	2.18	0.44
1:F:144:PHE:CE1	1:F:156:VAL:HG11	2.52	0.44
1:F:72:PHE:HB3	1:F:76:THR:HG21	1.99	0.44
1:G:18:ASN:N	1:G:18:ASN:OD1	2.50	0.44
1:G:205:HIS:O	1:G:206:ASN:CB	2.66	0.44
1:G:293:LEU:O	1:G:297:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:O	1:B:363:PRO:HA	2.18	0.44
1:E:77:LYS:O	1:E:80:ASP:HB2	2.18	0.44
1:F:63:ARG:HH11	1:F:63:ARG:HG3	1.82	0.44
1:F:27:PRO:HB3	1:F:74:ALA:HB1	2.00	0.44
1:G:59:ASP:OD1	1:G:61:SER:O	2.36	0.44
1:B:157:LYS:HB2	1:B:157:LYS:HE3	1.77	0.44
1:F:132:LEU:H	1:F:132:LEU:HG	1.63	0.44
1:F:135:ILE:HD12	1:F:135:ILE:N	2.33	0.44
1:F:309:VAL:HG13	1:F:311:TYR:CD2	2.53	0.44
1:G:57:LEU:O	1:G:57:LEU:HD22	2.17	0.44
1:A:168:LEU:HD21	1:A:315:LYS:HD2	1.99	0.43
1:C:100:THR:HG22	1:C:101:ILE:N	2.32	0.43
1:G:199:LEU:HD13	1:G:200:GLU:N	2.33	0.43
1:G:295:LEU:HD12	1:G:298:VAL:CG1	2.48	0.43
1:G:53:ARG:HH21	1:G:57:LEU:CA	2.30	0.43
1:A:153:GLU:HG3	1:A:246:LYS:HE2	2.00	0.43
1:C:302:LEU:CB	1:C:359:ILE:HG22	2.45	0.43
1:E:205:HIS:O	1:E:206:ASN:HB3	2.18	0.43
1:F:168:LEU:HB2	1:F:182:LEU:HB2	1.99	0.43
1:F:178:VAL:HG22	1:F:178:VAL:O	2.18	0.43
1:F:309:VAL:O	1:F:311:TYR:N	2.51	0.43
1:F:19:ILE:CG2	1:F:360:LEU:HA	2.47	0.43
1:A:311:TYR:CE1	1:A:321:GLN:HG3	2.53	0.43
1:A:63:ARG:NH1	1:A:63:ARG:HG3	2.29	0.43
1:A:98:ASN:HB3	1:A:328:THR:HG23	2.00	0.43
1:B:264:VAL:HG21	1:B:320:LEU:HD11	1.99	0.43
1:B:311:TYR:CD1	1:B:321:GLN:HG3	2.53	0.43
1:B:327:ARG:HG3	1:B:362:LYS:O	2.18	0.43
1:C:270:GLU:HG2	1:C:271:ASN:H	1.83	0.43
1:C:322:ASP:O	1:C:328:THR:HB	2.19	0.43
1:E:158:VAL:HG13	1:E:204:VAL:HG21	2.00	0.43
1:F:128:GLU:OE2	1:F:141:HIS:NE2	2.51	0.43
1:F:144:PHE:CE2	1:F:206:ASN:C	2.92	0.43
1:A:109:THR:OG1	1:A:335:THR:HG22	2.18	0.43
1:B:116:GLU:HG2	4:B:801:DQ8:CAK	2.48	0.43
1:F:146:LYS:HB3	1:F:146:LYS:HE3	1.66	0.43
1:C:23:VAL:HG21	1:C:68:PHE:CE2	2.53	0.43
1:C:306:THR:HG23	1:C:307:PRO:CD	2.33	0.43
1:E:106:GLN:HE22	1:E:342:ASN:HB3	1.84	0.43
1:E:156:VAL:CG2	1:E:204:VAL:O	2.67	0.43
1:F:309:VAL:HA	1:F:310:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:VAL:O	1:E:89:ILE:N	2.51	0.43
1:G:196:ILE:O	1:G:196:ILE:HG13	2.18	0.43
1:A:202:ILE:HD12	1:A:202:ILE:N	2.34	0.43
4:A:801:DQ8:CAL	4:A:801:DQ8:CAP	2.95	0.43
1:B:293:LEU:HD11	1:B:297:ARG:NH1	2.34	0.43
1:C:19:ILE:HD11	1:C:359:ILE:HG13	1.98	0.43
1:G:124:GLU:HG2	1:G:125:TYR:CE2	2.54	0.43
1:G:293:LEU:HD21	1:G:297:ARG:HH21	1.84	0.43
4:E:801:DQ8:HAK	4:E:801:DQ8:HAA1	1.83	0.43
1:F:91:ASP:O	1:F:94:ILE:N	2.52	0.43
1:A:230:ALA:O	1:A:234:ARG:HB2	2.19	0.43
1:A:99:CYS:O	1:A:261:LEU:CD1	2.65	0.43
1:D:26:ARG:CG	1:D:26:ARG:NH1	2.81	0.43
1:E:202:ILE:HG13	1:E:213:ILE:HD11	2.00	0.43
1:F:102:PHE:HB3	1:F:264:VAL:HG13	1.98	0.43
1:A:168:LEU:HD22	1:A:168:LEU:N	2.34	0.42
1:C:210:VAL:HG12	1:C:211:TYR:N	2.34	0.42
1:E:170:ASP:C	1:E:170:ASP:OD1	2.57	0.42
1:E:49:GLU:HG2	1:E:67:THR:HG22	2.01	0.42
1:F:216:LYS:NZ	1:F:217:GLY:N	2.66	0.42
1:F:307:PRO:O	1:F:308:HIS:C	2.57	0.42
1:G:102:PHE:CZ	1:G:295:LEU:HD21	2.54	0.42
1:G:79:ILE:HG12	1:G:83:ARG:CZ	2.49	0.42
1:E:156:VAL:CG2	1:E:204:VAL:HB	2.46	0.42
1:F:113:PHE:CD1	1:F:113:PHE:C	2.91	0.42
1:F:221:ARG:O	1:F:222:THR:C	2.56	0.42
1:G:231:TYR:H	1:G:231:TYR:HD1	1.63	0.42
1:A:47:ARG:HG3	1:A:47:ARG:HH11	1.84	0.42
1:D:26:ARG:HD3	1:D:109:THR:HA	2.00	0.42
1:G:196:ILE:HG12	1:G:199:LEU:HD23	2.00	0.42
1:G:43:CYS:HB3	1:G:71:VAL:CG1	2.49	0.42
1:A:126:THR:O	1:A:127:TRP:C	2.57	0.42
1:B:357:LYS:HB3	1:B:357:LYS:HE2	1.77	0.42
1:C:165:ASN:O	1:C:166:GLU:HB2	2.19	0.42
1:E:162:GLU:HG3	1:E:171:LEU:HD21	2.02	0.42
1:G:78:GLN:O	1:G:81:VAL:CG2	2.68	0.42
1:C:59:ASP:C	1:C:59:ASP:OD1	2.58	0.42
1:F:123:GLU:OE1	1:F:124:GLU:N	2.52	0.42
1:G:169:PHE:CD1	1:G:169:PHE:N	2.87	0.42
1:G:336:ILE:HD13	1:G:336:ILE:HA	1.61	0.42
1:G:91:ASP:HA	1:G:94:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HE1	1:A:156:VAL:CG1	2.23	0.42
1:C:143:ILE:CD1	1:C:243:ILE:HD11	2.49	0.42
1:D:236:HIS:HE2	1:D:291:SER:HB3	1.85	0.42
1:B:303:VAL:CG2	1:B:304:GLU:HG3	2.50	0.42
1:D:64:LYS:HE2	1:D:66:TYR:CZ	2.53	0.42
1:F:102:PHE:CD1	1:F:102:PHE:O	2.72	0.42
1:B:102:PHE:CE1	1:B:332:ILE:CG1	2.98	0.42
1:B:362:LYS:HA	1:B:363:PRO:HD3	1.82	0.42
1:C:170:ASP:OD2	1:C:199:LEU:HA	2.20	0.42
1:C:212:GLN:HB2	1:C:212:GLN:HE21	1.68	0.42
1:E:93:VAL:O	1:E:259:GLY:HA3	2.20	0.42
1:F:306:THR:CB	1:F:307:PRO:CD	2.96	0.42
4:F:801:DQ8:HAK	4:F:801:DQ8:HAA1	1.77	0.42
1:G:78:GLN:HB2	1:G:138:ARG:NH2	2.35	0.42
1:A:33:ARG:NH1	1:A:33:ARG:HG2	2.34	0.42
1:A:309:VAL:HB	1:A:311:TYR:CE2	2.55	0.42
1:E:195:ILE:HG13	1:E:195:ILE:O	2.20	0.42
1:E:26:ARG:HG3	1:E:26:ARG:H	1.65	0.42
1:E:292:LEU:HA	1:E:292:LEU:HD12	1.77	0.42
1:E:72:PHE:CD2	1:E:76:THR:HG21	2.55	0.42
1:G:149:ASP:N	1:G:149:ASP:OD1	2.44	0.42
1:G:155:SER:HB2	1:G:244:HIS:ND1	2.35	0.42
1:D:134:GLY:O	1:D:138:ARG:HG3	2.20	0.41
1:D:158:VAL:HA	1:D:240:SER:O	2.19	0.41
1:D:214:LEU:HD13	4:D:801:DQ8:CAJ	2.50	0.41
1:F:159:SER:HA	1:F:172:LEU:HD12	2.02	0.41
1:F:23:VAL:HG21	1:F:68:PHE:CE2	2.54	0.41
1:A:136:ILE:HB	1:A:137:PRO:HD3	2.02	0.41
1:C:33:ARG:NH1	1:G:179:SER:OG	2.54	0.41
1:C:357:LYS:H	1:C:357:LYS:HG3	1.66	0.41
1:C:362:LYS:N	1:C:362:LYS:CD	2.79	0.41
1:F:143:ILE:HD12	1:F:143:ILE:HA	1.87	0.41
1:F:350:LEU:HD23	1:F:350:LEU:HA	1.82	0.41
1:G:182:LEU:HA	1:G:182:LEU:HD12	1.58	0.41
1:G:160:LEU:HD22	4:G:801:DQ8:HAA2	2.02	0.41
1:A:144:PHE:O	1:A:147:LEU:N	2.53	0.41
1:A:322:ASP:O	1:A:328:THR:OG1	2.37	0.41
1:D:162:GLU:HG2	1:D:237:SER:HB3	2.03	0.41
1:E:294:THR:HG22	1:E:317:THR:HG21	2.01	0.41
1:E:293:LEU:HD23	1:E:297:ARG:NH1	2.35	0.41
1:F:161:LEU:CD1	1:F:161:LEU:C	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HB2	1:A:207:LYS:CD	2.51	0.41
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.66	0.41
1:C:261:LEU:HG	1:C:263:LEU:HD21	2.03	0.41
1:F:144:PHE:HE1	1:F:156:VAL:HG11	1.84	0.41
1:F:90:LEU:HD12	1:F:90:LEU:C	2.37	0.41
1:G:161:LEU:CD1	1:G:162:GLU:N	2.82	0.41
1:A:94:ILE:O	1:A:94:ILE:HG22	2.21	0.41
1:B:247:GLU:CD	1:B:255:LEU:O	2.59	0.41
4:B:801:DQ8:HAK	4:B:801:DQ8:HAA1	1.87	0.41
1:D:77:LYS:HA	1:D:77:LYS:HD2	1.82	0.41
1:G:271:ASN:OD1	1:G:271:ASN:O	2.38	0.41
1:G:305:ARG:HD3	1:G:306:THR:N	2.36	0.41
1:G:312:ARG:CG	1:G:313:GLU:N	2.79	0.41
1:A:330:THR:CG2	1:A:331:SER:H	2.33	0.41
1:A:64:LYS:HE2	1:A:64:LYS:HB3	1.88	0.41
1:B:92:GLU:OE2	1:B:329:ARG:CZ	2.68	0.41
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.77	0.41
1:D:51:SER:HB2	1:D:65:THR:OG1	2.21	0.41
1:D:64:LYS:HB3	1:D:64:LYS:HE3	1.63	0.41
1:F:124:GLU:O	1:F:125:TYR:CD1	2.73	0.41
1:E:61:SER:O	1:F:64:LYS:HA	2.21	0.41
1:A:120:SER:HA	1:A:121:PRO:HD3	1.94	0.41
4:B:801:DQ8:HAS1	4:B:801:DQ8:HAQ	2.01	0.41
1:C:119:ARG:HA	1:C:130:ASP:OD2	2.21	0.41
1:C:206:ASN:HD21	1:C:208:ASP:HB2	1.75	0.41
1:C:292:LEU:HA	1:C:292:LEU:HD12	1.76	0.41
1:D:212:GLN:CD	1:D:212:GLN:N	2.74	0.41
4:E:801:DQ8:HAQ	4:E:801:DQ8:HAS1	2.00	0.41
1:F:127:TRP:CE3	1:F:127:TRP:O	2.74	0.41
1:F:222:THR:O	1:F:226:THR:HG23	2.20	0.41
1:F:93:VAL:O	1:F:96:GLY:N	2.40	0.41
1:A:166:GLU:OE2	1:A:291:SER:OG	2.29	0.41
1:B:143:ILE:HD13	1:B:243:ILE:HD11	2.01	0.41
1:B:102:PHE:CE1	1:B:332:ILE:CD1	2.97	0.41
1:F:263:LEU:N	1:F:263:LEU:HD23	2.36	0.41
1:F:266:LEU:HD22	1:F:316:LEU:HD21	2.03	0.41
1:C:309:VAL:HG11	1:C:311:TYR:CZ	2.56	0.41
1:F:171:LEU:HD13	1:F:171:LEU:HA	1.77	0.41
1:F:291:SER:HB3	1:F:316:LEU:HB3	2.03	0.41
1:A:126:THR:O	1:A:129:GLU:N	2.54	0.41
1:C:82:TYR:CD1	1:C:86:VAL:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLU:O	1:D:125:TYR:N	2.54	0.41
1:D:168:LEU:HB2	1:D:182:LEU:HB2	2.03	0.41
1:D:83:ARG:HA	1:D:87:CYS:SG	2.61	0.41
1:G:162:GLU:OE2	1:G:231:TYR:OH	2.37	0.41
1:G:144:PHE:HE2	1:G:206:ASN:O	2.03	0.41
1:A:20:GLN:O	1:A:331:SER:HA	2.21	0.40
1:B:288:ILE:HD12	1:B:288:ILE:O	2.20	0.40
1:D:120:SER:N	1:D:130:ASP:OD2	2.43	0.40
1:F:69:ASP:O	1:F:70:MET:HG3	2.21	0.40
1:G:237:SER:HB3	1:G:265:ASP:HB3	2.03	0.40
1:D:127:TRP:CE2	1:D:128:GLU:HG3	2.56	0.40
1:F:234:ARG:HD3	1:F:288:ILE:HD11	2.02	0.40
1:E:59:ASP:OD2	1:F:64:LYS:NZ	2.55	0.40
1:G:292:LEU:HA	1:G:292:LEU:HD12	1.73	0.40
1:B:48:LYS:HE2	1:B:48:LYS:HB3	1.80	0.40
1:C:266:LEU:CD2	1:C:316:LEU:HD21	2.52	0.40
1:D:229:ASN:O	1:D:230:ALA:HB3	2.21	0.40
1:F:112:THR:HG22	1:F:113:PHE:N	2.36	0.40
1:F:242:THR:HB	1:F:260:LYS:HG3	2.03	0.40
1:F:82:TYR:C	1:F:82:TYR:CD1	2.95	0.40
1:A:103:ALA:HB1	1:A:111:LYS:CB	2.51	0.40
1:A:192:ARG:NH2	1:A:327:ARG:HG3	2.37	0.40
1:A:86:VAL:O	1:A:89:ILE:N	2.54	0.40
1:A:93:VAL:HG11	1:A:261:LEU:HB2	2.02	0.40
1:B:312:ARG:HD3	1:B:312:ARG:HA	1.86	0.40
1:D:111:LYS:HB2	2:D:601:ADP:O2B	2.20	0.40
1:E:143:ILE:HG23	1:E:243:ILE:HD13	2.04	0.40
1:F:199:LEU:HD12	1:F:200:GLU:N	2.37	0.40
1:A:114:THR:O	1:A:135:ILE:HG13	2.22	0.40
1:B:18:ASN:HA	1:B:360:LEU:HA	2.03	0.40
1:C:293:LEU:CD2	1:C:297:ARG:NH2	2.85	0.40
1:C:308:HIS:HB3	7:D:2024:HOH:O	2.21	0.40
1:D:137:PRO:HD3	4:D:801:DQ8:HAJ	2.02	0.40
1:E:130:ASP:OD1	1:E:131:PRO:HD2	2.22	0.40
1:F:184:MET:CE	1:F:319:ILE:HG13	2.52	0.40
1:F:136:ILE:CG2	1:F:239:PHE:CE2	3.05	0.40
1:F:243:ILE:N	1:F:259:GLY:O	2.44	0.40
1:G:301:ALA:HA	1:G:304:GLU:O	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/368 (86%)	300 (95%)	17 (5%)	0	100	100
1	B	319/368 (87%)	308 (97%)	11 (3%)	0	100	100
1	C	320/368 (87%)	302 (94%)	17 (5%)	1 (0%)	44	75
1	D	317/368 (86%)	303 (96%)	14 (4%)	0	100	100
1	E	315/368 (86%)	300 (95%)	15 (5%)	0	100	100
1	F	314/368 (85%)	286 (91%)	27 (9%)	1 (0%)	44	75
1	G	312/368 (85%)	277 (89%)	33 (11%)	2 (1%)	28	59
All	All	2214/2576 (86%)	2076 (94%)	134 (6%)	4 (0%)	51	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	206	ASN
1	G	97	TYR
1	C	190	ASN
1	F	307	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/322 (88%)	256 (90%)	28 (10%)	9	24
1	B	288/322 (89%)	260 (90%)	28 (10%)	9	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	287/322 (89%)	255 (89%)	32 (11%)	7	19
1	D	284/322 (88%)	262 (92%)	22 (8%)	15	36
1	E	281/322 (87%)	248 (88%)	33 (12%)	6	17
1	F	279/322 (87%)	233 (84%)	46 (16%)	2	7
1	G	269/322 (84%)	206 (77%)	63 (23%)	1	2
All	All	1972/2254 (88%)	1720 (87%)	252 (13%)	5	13

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	51	SER
1	A	63	ARG
1	A	111	LYS
1	A	126	THR
1	A	142	GLN
1	A	161	LEU
1	A	178	VAL
1	A	182	LEU
1	A	189	ARG
1	A	197	LYS
1	A	208	ASP
1	A	220	LYS
1	A	227	LEU
1	A	237	SER
1	A	240	SER
1	A	255	LEU
1	A	289	ASN
1	A	291	SER
1	A	298	VAL
1	A	306	THR
1	A	328	THR
1	A	341	LEU
1	A	343	LEU
1	A	348	SER
1	A	351	GLU
1	A	357	LYS
1	A	360	LEU
1	B	18	ASN
1	B	19	ILE

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Mol	Chain	Res	Type
1	B	20	GLN
1	B	64	LYS
1	B	102	PHE
1	B	111	LYS
1	B	119	ARG
1	B	123	GLU
1	B	126	THR
1	B	128	GLU
1	B	141	HIS
1	B	161	LEU
1	B	178	VAL
1	B	184	MET
1	B	207	LYS
1	B	220	LYS
1	B	227	LEU
1	B	233	SER
1	B	237	SER
1	B	247	GLU
1	B	255	LEU
1	B	288	ILE
1	B	289	ASN
1	B	291	SER
1	B	327	ARG
1	B	341	LEU
1	B	355	ARG
1	B	360	LEU
1	C	30	LEU
1	C	34	LYS
1	C	67	THR
1	C	94	ILE
1	C	119	ARG
1	C	126	THR
1	C	129	GLU
1	C	145[A]	GLU
1	C	145[B]	GLU
1	C	149	ASP
1	C	161	LEU
1	C	162	GLU
1	C	168	LEU
1	C	178	VAL
1	C	186	ASP
1	C	189	ARG

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Mol	Chain	Res	Type
1	C	190	ASN
1	C	203	THR
1	C	206	ASN
1	C	207	LYS
1	C	212	GLN
1	C	227	LEU
1	C	234	ARG
1	C	308	HIS
1	C	320	LEU
1	C	324	LEU
1	C	337	SER
1	C	340	SER
1	C	341	LEU
1	C	359	ILE
1	C	360	LEU
1	C	362	LYS
1	D	19	ILE
1	D	36	SER
1	D	64	LYS
1	D	79	ILE
1	D	90	LEU
1	D	93	VAL
1	D	126	THR
1	D	168	LEU
1	D	206	ASN
1	D	207	LYS
1	D	220	LYS
1	D	227	LEU
1	D	229	ASN
1	D	232	SER
1	D	237	SER
1	D	291	SER
1	D	293	LEU
1	D	303	VAL
1	D	309	VAL
1	D	337	SER
1	D	341	LEU
1	D	351	GLU
1	E	19	ILE
1	E	20	GLN
1	E	26	ARG
1	E	33	ARG

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Mol	Chain	Res	Type
1	E	36	SER
1	E	59	ASP
1	E	84	SER
1	E	92	GLU
1	E	97	TYR
1	E	111	LYS
1	E	125	TYR
1	E	142	GLN
1	E	145	GLU
1	E	147	LEU
1	E	152	THR
1	E	154	PHE
1	E	184	MET
1	E	185	PHE
1	E	191	LYS
1	E	195	ILE
1	E	202	ILE
1	E	212	GLN
1	E	216	LYS
1	E	222	THR
1	E	227	LEU
1	E	237	SER
1	E	258	ILE
1	E	288	ILE
1	E	293	LEU
1	E	312	ARG
1	E	348	SER
1	E	355	ARG
1	E	361	ASN
1	F	19	ILE
1	F	20	GLN
1	F	26	ARG
1	F	32	GLU
1	F	36	SER
1	F	51	SER
1	F	79	ILE
1	F	86	VAL
1	F	89	ILE
1	F	90	LEU
1	F	102	PHE
1	F	112	THR
1	F	115	MET

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Mol	Chain	Res	Type
1	F	120	SER
1	F	123	GLU
1	F	132	LEU
1	F	141	HIS
1	F	148	THR
1	F	154	PHE
1	F	168	LEU
1	F	171	LEU
1	F	181	ARG
1	F	194	VAL
1	F	195	ILE
1	F	204	VAL
1	F	213	ILE
1	F	216	LYS
1	F	220	LYS
1	F	227	LEU
1	F	239	PHE
1	F	242	THR
1	F	243	ILE
1	F	244	HIS
1	F	257	LYS
1	F	265	ASP
1	F	271	ASN
1	F	293	LEU
1	F	306	THR
1	F	308	HIS
1	F	312	ARG
1	F	323	SER
1	F	341	LEU
1	F	351	GLU
1	F	352	TYR
1	F	360	LEU
1	F	361	ASN
1	G	18	ASN
1	G	21	VAL
1	G	34	LYS
1	G	39	SER
1	G	41	VAL
1	G	44	ASP
1	G	47	ARG
1	G	53	ARG
1	G	57	LEU

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Mol	Chain	Res	Type
1	G	67	THR
1	G	69	ASP
1	G	79	ILE
1	G	81	VAL
1	G	86	VAL
1	G	89	ILE
1	G	98	ASN
1	G	100	THR
1	G	102	PHE
1	G	104	TYR
1	G	107	THR
1	G	122	ASN
1	G	128	GLU
1	G	149	ASP
1	G	155	SER
1	G	158	VAL
1	G	159	SER
1	G	161	LEU
1	G	166	GLU
1	G	168	LEU
1	G	181	ARG
1	G	182	LEU
1	G	184	MET
1	G	185	PHE
1	G	186	ASP
1	G	189	ARG
1	G	190	ASN
1	G	196	ILE
1	G	199	LEU
1	G	200	GLU
1	G	205	HIS
1	G	220	LYS
1	G	223	THR
1	G	226	THR
1	G	227	LEU
1	G	228	MET
1	G	233	SER
1	G	234	ARG
1	G	243	ILE
1	G	291	SER
1	G	292	LEU
1	G	293	LEU

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Mol	Chain	Res	Type
1	G	294	THR
1	G	298	VAL
1	G	299	ILE
1	G	302	LEU
1	G	306	THR
1	G	316	LEU
1	G	321	GLN
1	G	329	ARG
1	G	336	ILE
1	G	340	SER
1	G	347	LEU
1	G	350	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	20	GLN
1	G	18	ASN
1	G	262	ASN
1	G	354	HIS
1	G	358	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 21 are monoatomic - leaving 15 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	25,29,29	1.09	2 (8%)	24,45,45	1.71	4 (16%)
4	DQ8	A	801	-	28,28,28	0.90	2 (7%)	37,38,38	1.06	2 (5%)
2	ADP	B	601	3	25,29,29	1.05	2 (8%)	24,45,45	1.79	5 (20%)
4	DQ8	B	801	-	28,28,28	0.69	0	37,38,38	0.99	2 (5%)
2	ADP	C	601	3	25,29,29	1.20	2 (8%)	24,45,45	2.06	7 (29%)
4	DQ8	C	801	-	28,28,28	0.85	1 (3%)	37,38,38	1.26	6 (16%)
6	SO4	D	1362	-	4,4,4	0.28	0	6,6,6	0.35	0
2	ADP	D	601	3	25,29,29	1.04	2 (8%)	24,45,45	1.71	4 (16%)
4	DQ8	D	801	-	28,28,28	1.07	2 (7%)	37,38,38	1.30	4 (10%)
2	ADP	E	601	3	25,29,29	1.10	1 (4%)	24,45,45	1.91	5 (20%)
4	DQ8	E	801	-	28,28,28	0.72	1 (3%)	37,38,38	1.03	3 (8%)
2	ADP	F	601	3	25,29,29	1.10	1 (4%)	24,45,45	1.49	4 (16%)
4	DQ8	F	801	-	28,28,28	0.80	1 (3%)	37,38,38	1.03	2 (5%)
2	ADP	G	601	3	25,29,29	1.14	3 (12%)	24,45,45	1.90	4 (16%)
4	DQ8	G	801	-	28,28,28	0.96	2 (7%)	37,38,38	1.18	4 (10%)

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	-	0/12/32/32	0/3/3/3
4	DQ8	A	801	-	-	0/27/27/27	0/3/3/3
2	ADP	B	601	3	-	0/12/32/32	0/3/3/3
4	DQ8	B	801	-	-	0/27/27/27	0/3/3/3
2	ADP	C	601	3	-	0/12/32/32	0/3/3/3
4	DQ8	C	801	-	-	0/27/27/27	0/3/3/3
6	SO4	D	1362	-	-	0/0/0/0	0/0/0/0
2	ADP	D	601	3	-	0/12/32/32	0/3/3/3
4	DQ8	D	801	-	-	0/27/27/27	0/3/3/3
2	ADP	E	601	3	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DQ8	E	801	-	-	0/27/27/27	0/3/3/3
2	ADP	F	601	3	-	0/12/32/32	0/3/3/3
4	DQ8	F	801	-	-	0/27/27/27	0/3/3/3
2	ADP	G	601	3	-	0/12/32/32	0/3/3/3
4	DQ8	G	801	-	-	0/27/27/27	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	801	DQ8	CAZ-SAT	-3.32	1.83	1.87
2	C	601	ADP	C2'-C1'	-2.82	1.49	1.53
2	A	601	ADP	C2'-C1'	-2.64	1.49	1.53
4	C	801	DQ8	CAZ-SAT	-2.55	1.84	1.87
4	A	801	DQ8	CAZ-SAT	-2.46	1.84	1.87
4	G	801	DQ8	CAZ-SAT	-2.35	1.84	1.87
2	B	601	ADP	C2'-C1'	-2.29	1.50	1.53
4	G	801	DQ8	CAZ-CAW	-2.18	1.50	1.54
4	E	801	DQ8	CAS-SAT	2.07	1.86	1.81
2	G	601	ADP	C2-N3	2.09	1.35	1.32
2	G	601	ADP	O4'-C1'	2.19	1.44	1.41
4	F	801	DQ8	CAS-SAT	2.23	1.86	1.81
4	D	801	DQ8	CAS-SAT	2.23	1.86	1.81
2	D	601	ADP	C5-C4	2.26	1.45	1.40
2	D	601	ADP	O4'-C1'	2.36	1.44	1.41
4	A	801	DQ8	CAS-SAT	2.41	1.86	1.81
2	B	601	ADP	C5-C4	2.51	1.46	1.40
2	A	601	ADP	C5-C4	2.95	1.47	1.40
2	E	601	ADP	C5-C4	3.06	1.47	1.40
2	C	601	ADP	C5-C4	3.20	1.47	1.40
2	F	601	ADP	C5-C4	3.38	1.48	1.40
2	G	601	ADP	C5-C4	3.42	1.48	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	ADP	N3-C2-N1	-6.80	122.94	128.86
2	C	601	ADP	N3-C2-N1	-6.06	123.58	128.86
2	G	601	ADP	N3-C2-N1	-5.55	124.02	128.86
2	B	601	ADP	N3-C2-N1	-5.32	124.22	128.86
2	A	601	ADP	N3-C2-N1	-4.81	124.67	128.86
2	G	601	ADP	C5'-C4'-C3'	-4.47	98.25	115.29
2	F	601	ADP	N3-C2-N1	-4.32	125.10	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ADP	N3-C2-N1	-4.04	125.34	128.86
2	C	601	ADP	O2'-C2'-C1'	-3.94	99.29	111.61
2	A	601	ADP	C4-C5-N7	-3.68	105.85	109.41
2	D	601	ADP	C4'-O4'-C1'	-3.18	106.38	109.77
2	B	601	ADP	C4-C5-N7	-2.91	106.60	109.41
2	F	601	ADP	C4-C5-N7	-2.89	106.61	109.41
2	D	601	ADP	C5'-C4'-C3'	-2.82	104.55	115.29
4	D	801	DQ8	CAH-CAN-CAX	-2.81	117.73	120.77
4	G	801	DQ8	CAP-CAY-CAZ	-2.76	115.75	121.06
4	G	801	DQ8	CAK-CAV-CAU	-2.65	115.28	120.86
4	C	801	DQ8	CAG-CAM-CAW	-2.60	117.96	120.77
4	C	801	DQ8	CAW-CAZ-CAX	-2.53	104.39	111.09
2	B	601	ADP	O2'-C2'-C1'	-2.52	103.72	111.61
4	C	801	DQ8	CAJ-CAK-CAV	-2.50	117.41	120.35
4	E	801	DQ8	CAW-CAZ-CAY	-2.47	104.55	111.09
2	C	601	ADP	C5'-C4'-C3'	-2.39	106.16	115.29
4	F	801	DQ8	CAO-CAX-CAZ	-2.34	116.55	121.06
2	C	601	ADP	C4-C5-N7	-2.33	107.16	109.41
4	C	801	DQ8	CAQ-CAV-CAU	-2.24	115.06	119.98
4	D	801	DQ8	CAE-CAI-CAO	-2.15	117.25	120.21
4	F	801	DQ8	CAH-CAN-CAX	-2.10	118.50	120.77
2	C	601	ADP	C1'-N9-C4	-2.09	123.02	126.64
2	E	601	ADP	C1'-N9-C4	-2.03	123.12	126.64
2	E	601	ADP	C4-C5-N7	-2.03	107.45	109.41
4	A	801	DQ8	CAQ-CAV-CAU	-2.02	115.56	119.98
2	E	601	ADP	O3B-PB-O2B	2.02	115.75	107.61
2	F	601	ADP	C2-N1-C6	2.03	122.32	118.77
4	G	801	DQ8	CAQ-CAY-CAZ	2.14	124.40	120.74
4	C	801	DQ8	CAM-CAW-CAL	2.14	121.19	117.94
4	A	801	DQ8	CAX-CAZ-CAY	2.16	116.79	111.09
4	B	801	DQ8	CAK-CAV-CAQ	2.16	121.77	119.23
4	E	801	DQ8	CAK-CAV-CAQ	2.24	121.87	119.23
4	D	801	DQ8	CAX-CAZ-CAY	2.25	117.04	111.09
2	G	601	ADP	O3B-PB-O2B	2.30	116.90	107.61
4	G	801	DQ8	CAX-CAZ-CAY	2.31	117.19	111.09
4	C	801	DQ8	CAX-CAZ-CAY	2.36	117.33	111.09
2	B	601	ADP	C4'-O4'-C1'	2.42	112.34	109.77
2	A	601	ADP	O2A-PA-O1A	2.42	124.78	112.28
2	G	601	ADP	N6-C6-N1	2.49	123.71	118.77
4	B	801	DQ8	CAX-CAZ-CAY	2.55	117.82	111.09
2	E	601	ADP	C2-N1-C6	2.63	123.38	118.77
2	A	601	ADP	O3B-PB-O1B	2.64	120.83	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	801	DQ8	CAX-CAZ-CAY	2.65	118.08	111.09
4	D	801	DQ8	CAK-CAV-CAQ	2.70	122.41	119.23
2	C	601	ADP	O3B-PB-O2B	2.72	118.59	107.61
2	F	601	ADP	O3B-PB-O2B	2.77	118.80	107.61
2	C	601	ADP	C2-N1-C6	2.95	123.94	118.77
2	B	601	ADP	O3B-PB-O1B	3.09	122.58	110.50
2	D	601	ADP	N6-C6-N1	3.21	125.13	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	DQ8	7	0
4	B	801	DQ8	8	0
2	C	601	ADP	4	0
4	C	801	DQ8	2	0
2	D	601	ADP	5	0
4	D	801	DQ8	4	0
2	E	601	ADP	5	0
4	E	801	DQ8	9	0
2	F	601	ADP	3	0
4	F	801	DQ8	7	0
2	G	601	ADP	2	0
4	G	801	DQ8	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	322/368 (87%)	0.52	39 (12%)	5 3	33, 54, 90, 112	0
1	B	324/368 (88%)	0.56	45 (13%)	3 2	34, 53, 92, 104	0
1	C	325/368 (88%)	0.27	28 (8%)	11 8	28, 50, 86, 113	0
1	D	322/368 (87%)	0.38	27 (8%)	12 8	28, 50, 92, 114	0
1	E	321/368 (87%)	0.72	53 (16%)	2 1	42, 67, 99, 119	0
1	F	319/368 (86%)	0.79	57 (17%)	2 1	41, 71, 106, 117	0
1	G	318/368 (86%)	1.11	72 (22%)	1 1	46, 81, 122, 140	0
All	All	2251/2576 (87%)	0.62	321 (14%)	3 2	28, 61, 105, 140	0

All (321) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	309	VAL	8.7
1	G	308	HIS	8.5
1	G	58	ALA	7.5
1	G	307	PRO	6.9
1	E	149	ASP	6.9
1	G	359	ILE	6.7
1	G	102	PHE	6.6
1	D	256	VAL	6.3
1	A	256	VAL	6.2
1	F	148	THR	6.0
1	A	149	ASP	5.9
1	G	191	LYS	5.8
1	F	363	PRO	5.7
1	B	152	THR	5.5
1	F	149	ASP	5.5
1	G	193	GLY	5.5
1	B	255	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	364	GLU	5.4
1	E	263	LEU	5.4
1	G	363	PRO	5.4
1	G	325	GLY	5.3
1	D	255	LEU	5.3
1	B	149	ASP	5.2
1	B	129	GLU	5.2
1	G	67	THR	5.2
1	A	101	ILE	5.2
1	G	190	ASN	5.1
1	G	264	VAL	5.1
1	A	102	PHE	5.1
1	E	186	ASP	5.0
1	E	150	ASN	5.0
1	A	264	VAL	4.8
1	C	365	VAL	4.8
1	F	102	PHE	4.8
1	G	188	PRO	4.8
1	B	151	GLY	4.6
1	B	189	ARG	4.6
1	E	153	GLU	4.6
1	A	188	PRO	4.5
1	G	332	ILE	4.5
1	B	148	THR	4.5
1	G	56	GLY	4.5
1	G	303	VAL	4.5
1	F	301	ALA	4.4
1	F	326	GLY	4.4
1	B	264	VAL	4.4
1	B	102	PHE	4.4
1	G	63	ARG	4.3
1	A	153	GLU	4.3
1	G	192	ARG	4.3
1	G	45	PRO	4.2
1	F	263	LEU	4.2
1	G	328	THR	4.2
1	E	360	LEU	4.2
1	A	238	VAL	4.1
1	A	257	LYS	4.1
1	F	155	SER	4.1
1	E	239	PHE	4.1
1	B	238	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	263	LEU	4.0
1	C	237	SER	4.0
1	G	306	THR	4.0
1	B	124	GLU	4.0
1	F	101	ILE	4.0
1	A	255	LEU	3.9
1	A	263	LEU	3.9
1	C	153	GLU	3.9
1	E	307	PRO	3.9
1	D	258	ILE	3.9
1	B	147	LEU	3.8
1	B	361	ASN	3.8
1	E	245	MET	3.8
1	F	238	VAL	3.8
1	E	332	ILE	3.8
1	G	57	LEU	3.8
1	G	103	ALA	3.8
1	G	329	ARG	3.8
1	G	334	ALA	3.8
1	E	122	ASN	3.8
1	G	360	LEU	3.8
1	B	150	ASN	3.8
1	E	262	ASN	3.8
1	G	115	MET	3.8
1	E	256	VAL	3.7
1	E	102	PHE	3.7
1	F	262	ASN	3.7
1	G	327	ARG	3.7
1	G	304	GLU	3.7
1	F	308	HIS	3.7
1	G	238	VAL	3.7
1	E	257	LYS	3.7
1	D	358	ASN	3.7
1	B	101	ILE	3.7
1	E	185	PHE	3.6
1	E	101	ILE	3.6
1	G	305	ARG	3.6
1	C	363	PRO	3.6
1	F	360	LEU	3.6
1	G	310	PRO	3.6
1	F	122	ASN	3.6
1	D	264	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	333	ILE	3.5
1	F	327	ARG	3.5
1	B	360	LEU	3.5
1	B	103	ALA	3.5
1	C	238	VAL	3.5
1	E	131	PRO	3.5
1	A	125	TYR	3.5
1	B	332	ILE	3.5
1	F	332	ILE	3.5
1	B	333	ILE	3.5
1	A	360	LEU	3.5
1	E	309	VAL	3.4
1	D	152	THR	3.4
1	G	44	ASP	3.4
1	B	100	THR	3.4
1	E	238	VAL	3.4
1	F	100	THR	3.4
1	A	100	THR	3.4
1	G	48	LYS	3.4
1	F	193	GLY	3.4
1	E	264	VAL	3.4
1	D	263	LEU	3.3
1	F	153[A]	GLU	3.3
1	F	264	VAL	3.3
1	A	152	THR	3.3
1	G	55	GLY	3.3
1	D	257	LYS	3.3
1	G	99	CYS	3.3
1	A	189	ARG	3.3
1	F	93	VAL	3.3
1	F	312	ARG	3.3
1	F	239	PHE	3.3
1	B	17	LYS	3.3
1	B	303	VAL	3.2
1	D	303	VAL	3.2
1	G	92	GLU	3.2
1	A	258	ILE	3.2
1	F	288	ILE	3.2
1	E	305	ARG	3.2
1	B	240	SER	3.2
1	B	362	LYS	3.2
1	F	362	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	240	SER	3.2
1	C	366	ASN	3.2
1	A	103	ALA	3.2
1	D	153	GLU	3.2
1	A	239	PHE	3.2
1	F	18	ASN	3.2
1	F	95	MET	3.2
1	B	192	ARG	3.2
1	F	307	PRO	3.1
1	D	254	GLU	3.1
1	E	126	THR	3.1
1	A	304	GLU	3.1
1	B	263	LEU	3.1
1	C	152	THR	3.1
1	E	129	GLU	3.1
1	A	262	ASN	3.1
1	G	101	ILE	3.1
1	G	322	ASP	3.1
1	C	151	GLY	3.1
1	G	23	VAL	3.1
1	F	154	PHE	3.1
1	G	46	VAL	3.0
1	C	362	LYS	3.0
1	F	103	ALA	3.0
1	G	293	LEU	3.0
1	A	333	ILE	3.0
1	G	151	GLY	3.0
1	F	304	GLU	3.0
1	D	151	GLY	3.0
1	E	333	ILE	3.0
1	G	47	ARG	3.0
1	C	263	LEU	3.0
1	E	301	ALA	3.0
1	E	246	LYS	2.9
1	G	185	PHE	2.9
1	C	122	ASN	2.9
1	F	129	GLU	2.9
1	G	258	ILE	2.9
1	C	288	ILE	2.9
1	E	100	THR	2.9
1	B	262	ASN	2.9
1	E	300	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	152	THR	2.9
1	F	45	PRO	2.9
1	E	151	GLY	2.9
1	C	101	ILE	2.9
1	E	190	ASN	2.8
1	B	363	PRO	2.8
1	B	331	SER	2.8
1	A	359	ILE	2.8
1	C	258	ILE	2.8
1	D	262	ASN	2.8
1	F	189	ARG	2.8
1	E	240	SER	2.8
1	F	257	LYS	2.8
1	A	151	GLY	2.8
1	D	246	LYS	2.7
1	E	135	ILE	2.7
1	A	303	VAL	2.7
1	G	59	ASP	2.7
1	E	152	THR	2.7
1	A	246	LYS	2.7
1	F	30	LEU	2.7
1	E	306	THR	2.7
1	G	149	ASP	2.7
1	B	239	PHE	2.7
1	F	237	SER	2.7
1	F	287	ASN	2.7
1	A	129	GLU	2.6
1	D	237	SER	2.6
1	D	240	SER	2.6
1	G	240	SER	2.6
1	G	301	ALA	2.6
1	G	239	PHE	2.6
1	A	148	THR	2.6
1	E	326	GLY	2.6
1	B	312	ARG	2.6
1	G	136	ILE	2.6
1	G	231	TYR	2.6
1	C	256	VAL	2.6
1	D	238	VAL	2.6
1	F	161	LEU	2.6
1	B	237	SER	2.6
1	D	148	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	333	ILE	2.5
1	B	125	TYR	2.5
1	F	331	SER	2.5
1	G	100	THR	2.5
1	B	261	LEU	2.5
1	D	288	ILE	2.5
1	B	191	LYS	2.5
1	E	361	ASN	2.5
1	G	189	ARG	2.5
1	A	332	ILE	2.5
1	D	186	ASP	2.5
1	F	136	ILE	2.5
1	F	150	ASN	2.5
1	C	161	LEU	2.4
1	F	266	LEU	2.4
1	A	191	LYS	2.4
1	F	131	PRO	2.4
1	D	360	LEU	2.4
1	A	331	SER	2.4
1	B	190	ASN	2.4
1	D	102	PHE	2.4
1	G	154	PHE	2.4
1	D	310	PRO	2.4
1	F	361	ASN	2.4
1	F	83	ARG	2.4
1	B	153	GLU	2.4
1	F	300	THR	2.4
1	G	230	ALA	2.4
1	D	101	ILE	2.4
1	E	234	ARG	2.4
1	G	311	TYR	2.4
1	E	293	LEU	2.4
1	E	187	ASP	2.4
1	F	192	ARG	2.4
1	E	103	ALA	2.4
1	E	136	ILE	2.4
1	G	355	ARG	2.4
1	E	191	LYS	2.3
1	F	123	GLU	2.3
1	B	307	PRO	2.3
1	C	240	SER	2.3
1	B	256	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	245	MET	2.3
1	G	148	THR	2.3
1	E	331	SER	2.3
1	E	304	GLU	2.3
1	C	150	ASN	2.3
1	C	262	ASN	2.3
1	C	287	ASN	2.3
1	G	135	ILE	2.3
1	A	330	THR	2.3
1	E	148	THR	2.3
1	G	194	VAL	2.3
1	B	121	PRO	2.2
1	B	247	GLU	2.2
1	G	312	ARG	2.2
1	C	154	PHE	2.2
1	G	124	GLU	2.2
1	B	246	LYS	2.2
1	G	271	ASN	2.2
1	G	300	THR	2.2
1	C	264	VAL	2.2
1	B	188	PRO	2.2
1	D	161	LEU	2.2
1	E	193	GLY	2.2
1	E	125	TYR	2.2
1	A	121	PRO	2.2
1	A	261	LEU	2.2
1	F	119	ARG	2.2
1	F	190	ASN	2.2
1	E	124	GLU	2.2
1	F	302	LEU	2.2
1	B	271	ASN	2.1
1	C	135	ILE	2.1
1	F	305	ARG	2.1
1	A	124	GLU	2.1
1	G	361	ASN	2.1
1	E	97	TYR	2.1
1	D	359	ILE	2.1
1	E	325	GLY	2.1
1	F	188	PRO	2.1
1	F	31	ALA	2.1
1	B	185	PHE	2.1
1	E	95	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	136	ILE	2.0
1	C	100	THR	2.0
1	A	185	PHE	2.0
1	F	185	PHE	2.0
1	E	189	ARG	2.0
1	G	297	ARG	2.0
1	A	150	ASN	2.0
1	D	361	ASN	2.0
1	C	149	ASP	2.0
1	C	102	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	DQ8	B	801	26/26	0.93	0.22	0.52	44,53,67,82	0
4	DQ8	C	801	26/26	0.92	0.22	0.42	39,49,61,83	0
4	DQ8	D	801	26/26	0.93	0.21	0.39	38,47,60,79	0
4	DQ8	A	801	26/26	0.90	0.23	0.34	43,54,63,85	0
4	DQ8	F	801	26/26	0.86	0.26	0.18	60,75,84,110	0
4	DQ8	G	801	26/26	0.93	0.22	0.10	49,57,68,85	0
2	ADP	C	601	27/27	0.98	0.16	-0.06	28,38,42,48	0
4	DQ8	E	801	26/26	0.88	0.22	-0.20	57,67,77,98	0
2	ADP	B	601	27/27	0.98	0.16	-0.46	35,42,48,58	0
2	ADP	E	601	27/27	0.97	0.16	-0.77	45,54,61,71	0
2	ADP	F	601	27/27	0.97	0.16	-0.89	45,55,70,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	D	601	27/27	0.98	0.14	-1.10	28,40,45,51	0
6	SO4	D	1362	5/5	0.97	0.12	-1.28	54,54,63,68	0
2	ADP	G	601	27/27	0.97	0.14	-1.31	46,54,59,64	0
2	ADP	A	601	27/27	0.98	0.13	-1.40	34,41,47,50	0
3	MG	D	701	1/1	0.97	0.18	-	35,35,35,35	0
5	CL	F	1364	1/1	0.95	0.14	-	89,89,89,89	0
5	CL	G	1364	1/1	0.43	0.34	-	106,106,106,106	0
5	CL	C	1369	1/1	0.92	0.11	-	97,97,97,97	0
5	CL	A	1365	1/1	0.89	0.08	-	95,95,95,95	0
5	CL	C	1367	1/1	0.97	0.29	-	62,62,62,62	0
5	CL	A	1367	1/1	0.95	0.18	-	73,73,73,73	0
3	MG	B	701	1/1	0.95	0.18	-	37,37,37,37	0
3	MG	C	701	1/1	0.93	0.23	-	40,40,40,40	0
5	CL	B	1364	1/1	0.96	0.32	-	80,80,80,80	0
3	MG	G	701	1/1	0.96	0.28	-	45,45,45,45	0
3	MG	E	701	1/1	0.97	0.20	-	50,50,50,50	0
3	MG	A	701	1/1	0.99	0.16	-	35,35,35,35	0
5	CL	E	1364	1/1	0.85	0.21	-	90,90,90,90	0
5	CL	D	1363	1/1	0.97	0.10	-	79,79,79,79	0
3	MG	F	701	1/1	0.94	0.15	-	50,50,50,50	0
5	CL	D	1364	1/1	0.83	0.12	-	77,77,77,77	0
5	CL	A	1366	1/1	0.71	0.15	-	89,89,89,89	0
5	CL	C	1368	1/1	0.97	0.10	-	56,56,56,56	0
5	CL	B	1365	1/1	0.83	0.09	-	78,78,78,78	0
5	CL	A	1364	1/1	0.89	0.08	-	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.