



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 02:41 am BST

PDB ID : 1HH4  
Title : Rac1-RhoGDI complex involved in NADPH oxidase activation  
Authors : Grizot, S.; Faure, J.; Fieschi, F.; Vignais, P.V.; Dagher, M.-C.; Pebay-Peyroula, E.  
Deposited on : 2000-12-20  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	1.8.5 (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

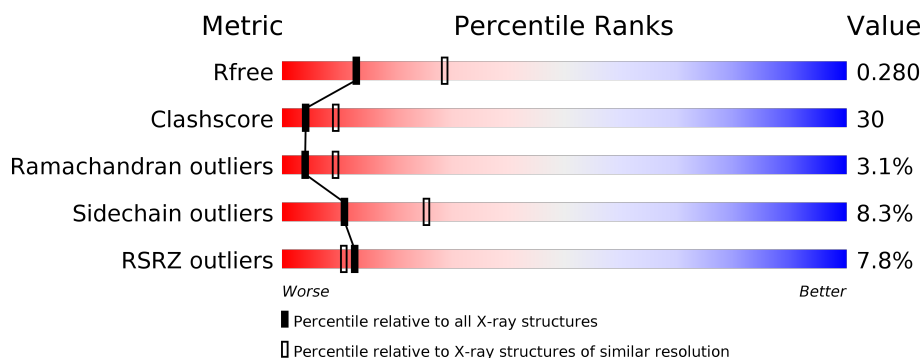
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	192	<div> <div>6%</div> <div>54%</div> <div>41%</div> <div>• •</div> </div>
1	B	192	<div> <div>7%</div> <div>43%</div> <div>50%</div> <div>5%</div> <div>•</div> </div>
2	D	204	<div> <div>9%</div> <div>48%</div> <div>39%</div> <div>•</div> <div>9%</div> </div>
2	E	204	<div> <div>7%</div> <div>44%</div> <div>39%</div> <div>5%</div> <div>•</div> <div>12%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GER	D	1502	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5908 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 RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1448	928	243	268	9			
1	B	189	Total	C	N	O	S	0	0	0
			1446	924	243	270	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	SER	PHE	cloning artifact	UNP P15154
A	1	PRO	MET	cloning artifact	UNP P15154
B	78	SER	PHE	cloning artifact	UNP P15154
B	1	PRO	MET	cloning artifact	UNP P15154

- Molecule 2 is a protein called RHO GDP-DISSOCIATION INHIBITOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	186	Total	C	N	O	S	0	0	0
			1445	912	245	285	3			
2	E	180	Total	C	N	O	S	0	0	0
			1441	915	243	279	4			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

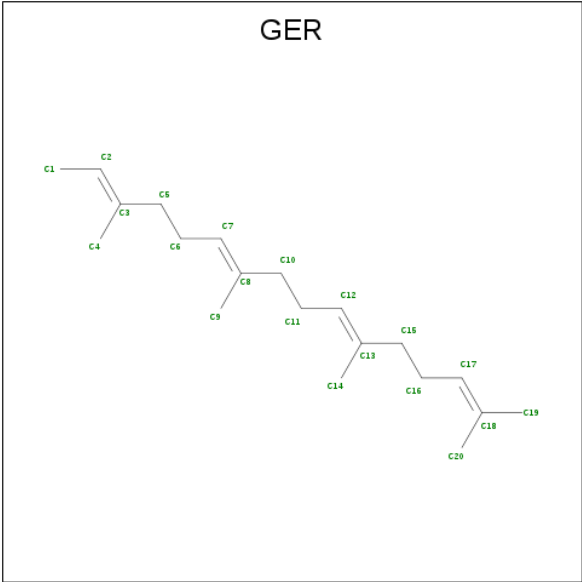


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0

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

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

- Molecule 5 is GERAN-8-YL GERAN (three-letter code: GER) (formula: C<sub>20</sub>H<sub>34</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C 20 20	0	0
5	E	1	Total C 20 20	0	0

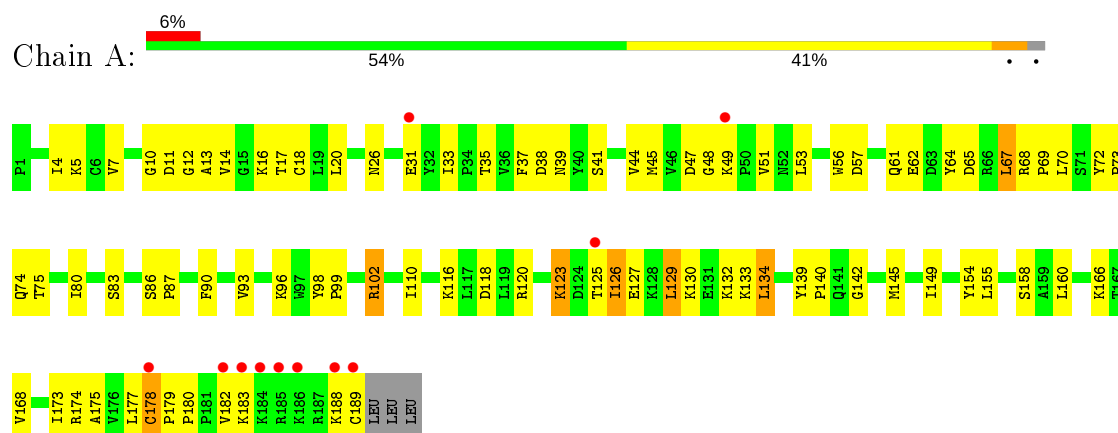
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	6	Total O 6 6	0	0
6	D	7	Total O 7 7	0	0
6	E	5	Total O 5 5	0	0

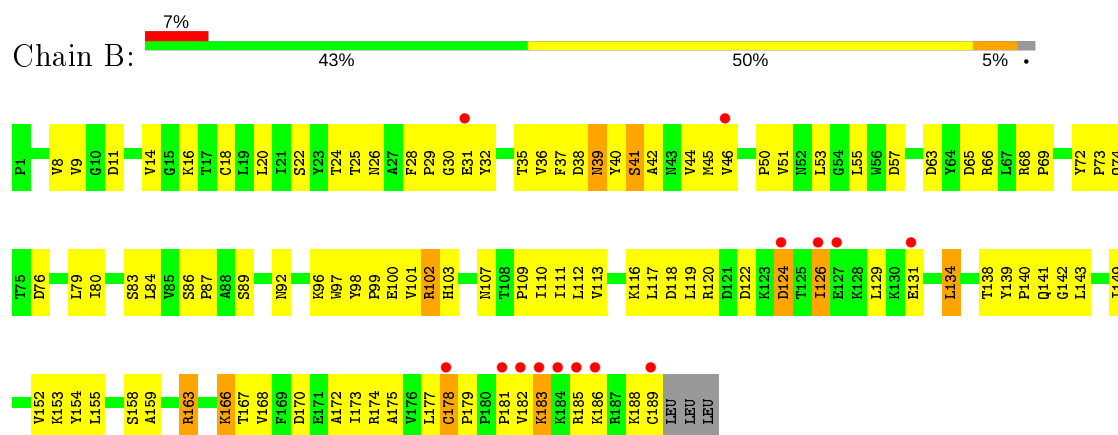
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

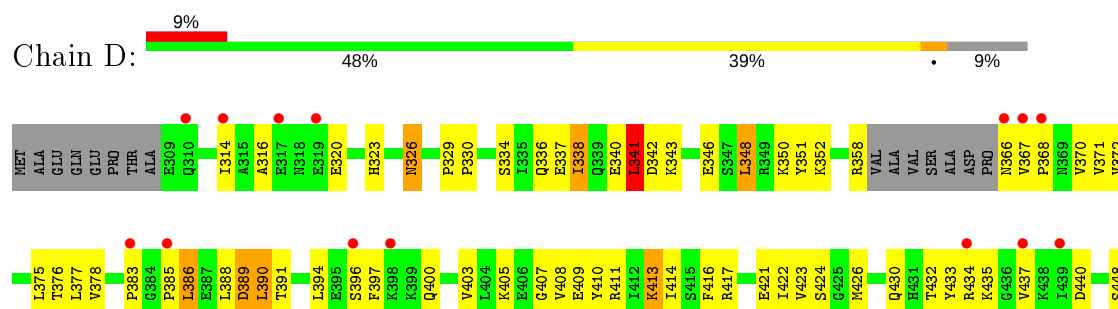
#### • Molecule 1: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1

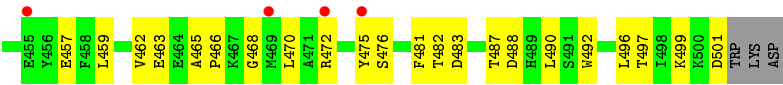


#### • Molecule 1: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1

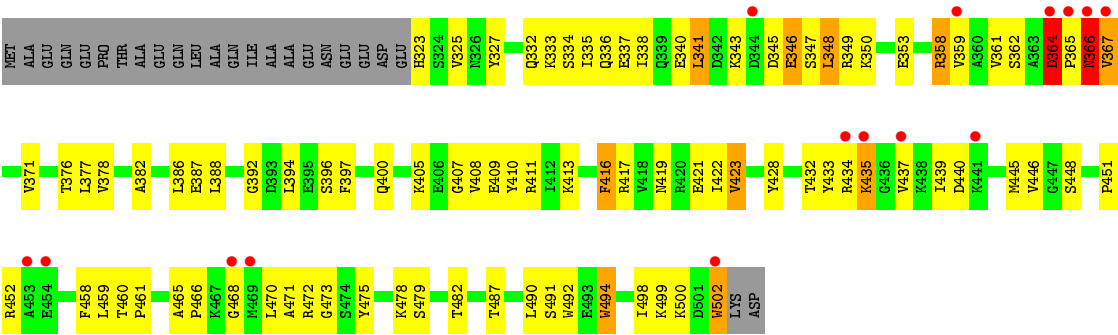


#### • Molecule 2: RHO GDP-DISSOCIATION INHIBITOR 1





● Molecule 2: RHO GDP-DISSOCIATION INHIBITOR 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.70 Å   88.70 Å   62.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.80 – 2.70 29.62 – 2.67	Depositor EDS
% Data completeness (in resolution range)	85.1 (19.80-2.70) 83.7 (29.62-2.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.68 Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.256   ,   0.280 0.256   ,   0.280	Depositor DCC
$R_{free}$ test set	1085 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8543e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.50	0/1480	0.71	0/2015
1	B	0.48	0/1478	0.77	0/2015
2	D	0.49	0/1472	0.75	1/1990 (0.1%)
2	E	0.44	0/1472	0.75	1/1989 (0.1%)
All	All	0.48	0/5902	0.74	2/8009 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	358	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	D	316	ALA	N-CA-CB	7.23	120.22	110.10

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	1448	0	1473	70	0
1	B	1446	0	1455	124	0
2	D	1445	0	1385	69	0
2	E	1441	0	1426	96	0
3	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	D	20	0	34	5	0
5	E	20	0	34	6	0
6	A	12	0	0	1	0
6	B	6	0	0	1	0
6	D	7	0	0	0	0
6	E	5	0	0	2	0
All	All	5908	0	5831	346	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 30.

All (346) 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:B:177:LEU:O	1:B:178:CYS:SG	1.99	1.19
1:A:64:TYR:CE1	2:D:341:LEU:HD12	1.89	1.07
2:E:472:ARG:NH1	2:E:500:LYS:HD2	1.73	1.04
1:B:65:ASP:HA	1:B:68:ARG:HH12	1.25	1.02
1:B:155:LEU:HD23	1:B:168:VAL:HA	1.42	0.98
1:A:102:ARG:HH12	1:A:110:ILE:HD11	1.26	0.98
2:E:466:PRO:HG3	5:E:1503:GER:H71	1.45	0.96
2:E:434:ARG:HH12	2:E:473:GLY:HA3	1.29	0.95
1:B:182:VAL:HG21	1:B:185:ARG:HH12	1.32	0.95
1:B:188:LYS:HA	2:E:466:PRO:HB3	1.49	0.94
1:B:183:LYS:N	1:B:183:LYS:HD2	1.83	0.91
2:D:430:GLN:HE22	5:D:1502:GER:H143	1.35	0.91
1:B:41:SER:HA	1:B:53:LEU:O	1.71	0.91
1:B:170:ASP:O	1:B:174:ARG:HG2	1.73	0.88
1:B:40:TYR:CE2	1:B:42:ALA:HB2	2.10	0.87
1:B:179:PRO:O	1:B:181:PRO:HD3	1.76	0.86
2:D:413:LYS:HE3	2:D:457:GLU:OE2	1.74	0.85
1:A:102:ARG:NH1	1:A:110:ILE:HD11	1.92	0.85
1:A:64:TYR:CZ	2:D:341:LEU:HD12	2.12	0.85
2:E:472:ARG:HH12	2:E:500:LYS:HD2	1.41	0.84
1:A:177:LEU:O	1:A:178:CYS:SG	2.37	0.82
1:A:123:LYS:HE3	1:A:123:LYS:HA	1.60	0.82
2:D:421:GLU:HG3	2:D:422:ILE:N	1.95	0.81
1:B:188:LYS:CB	2:E:466:PRO:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:434:ARG:HE	2:E:435:LYS:HE3	1.46	0.80
2:D:434:ARG:HG2	2:D:434:ARG:HH11	1.46	0.80
1:B:183:LYS:H	1:B:183:LYS:HD2	1.42	0.80
1:B:53:LEU:HD13	1:B:173:ILE:HD11	1.63	0.79
2:E:387:GLU:HG2	2:E:388:LEU:H	1.48	0.76
2:E:434:ARG:NH1	2:E:473:GLY:HA3	2.01	0.76
1:A:68:ARG:HB3	1:A:69:PRO:HD3	1.68	0.76
1:B:84:LEU:HD13	1:B:120:ARG:HD2	1.65	0.76
1:B:68:ARG:HB3	1:B:69:PRO:HD3	1.66	0.76
2:E:468:GLY:O	2:E:472:ARG:HB2	1.86	0.76
1:A:126:ILE:O	1:A:130:LYS:HB2	1.85	0.76
2:D:421:GLU:CG	2:D:422:ILE:H	1.99	0.75
1:A:35:THR:O	6:A:2002:HOH:O	2.05	0.75
2:E:325:VAL:HA	6:E:2001:HOH:O	1.87	0.75
2:D:334:SER:OG	2:D:337:GLU:HG3	1.87	0.74
2:E:437:VAL:O	2:E:439:ILE:HG23	1.87	0.74
2:D:421:GLU:HG3	2:D:422:ILE:H	1.50	0.74
2:D:403:VAL:HG11	2:D:499:LYS:HE3	1.69	0.73
2:E:353:GLU:CD	2:E:358:ARG:NH1	2.42	0.73
1:B:188:LYS:HA	2:E:466:PRO:CB	2.21	0.71
1:A:102:ARG:HH12	1:A:110:ILE:CD1	2.02	0.71
1:B:102:ARG:NH1	1:B:110:ILE:HD11	2.06	0.71
2:D:468:GLY:O	2:D:472:ARG:HB2	1.89	0.71
1:B:20:LEU:O	1:B:24:THR:HG23	1.91	0.71
1:A:90:PHE:CZ	1:A:145:MET:HG3	2.26	0.70
2:E:353:GLU:CD	2:E:358:ARG:HH12	1.93	0.70
1:B:182:VAL:HG21	1:B:185:ARG:NH1	2.06	0.70
1:B:175:ALA:O	1:B:179:PRO:HG2	1.92	0.70
2:D:411:ARG:HG3	2:D:459:LEU:HD22	1.73	0.70
2:D:348:LEU:O	2:D:352:LYS:HG3	1.91	0.70
1:B:139:TYR:N	1:B:140:PRO:HD2	2.08	0.69
2:E:353:GLU:OE2	2:E:358:ARG:NH1	2.26	0.68
2:D:421:GLU:CG	2:D:422:ILE:N	2.57	0.68
2:E:432:THR:HG21	5:E:1503:GER:H91	1.75	0.68
2:E:382:ALA:HB2	2:E:502:TRP:CZ2	2.29	0.67
1:B:98:TYR:O	1:B:102:ARG:HB2	1.94	0.67
2:D:433:TYR:HB2	2:D:476:SER:HB3	1.78	0.66
2:E:387:GLU:HG2	2:E:388:LEU:N	2.10	0.66
1:B:40:TYR:HE2	1:B:42:ALA:HB2	1.60	0.66
2:D:434:ARG:HG2	2:D:434:ARG:NH1	2.07	0.66
1:A:69:PRO:HA	1:A:72:TYR:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PRO:HG2	1:B:134:LEU:HD12	1.77	0.66
2:E:371:VAL:HG13	2:E:417:ARG:HB3	1.76	0.66
1:A:155:LEU:HD13	1:A:168:VAL:HA	1.78	0.65
2:D:375:LEU:HD21	2:D:481:PHE:HZ	1.61	0.65
1:A:87:PRO:HG2	1:A:134:LEU:HD12	1.79	0.65
2:E:334:SER:O	2:E:338:ILE:HG12	1.97	0.65
1:A:102:ARG:HB2	1:A:102:ARG:HH11	1.62	0.65
2:E:490:LEU:HG	2:E:491:SER:N	2.12	0.65
1:B:74:GLN:HA	1:B:74:GLN:NE2	2.12	0.64
1:A:41:SER:HA	1:A:53:LEU:O	1.98	0.64
2:D:430:GLN:NE2	5:D:1502:GER:H143	2.10	0.64
1:B:179:PRO:O	1:B:181:PRO:CD	2.46	0.64
1:A:126:ILE:O	1:A:130:LYS:HD2	1.98	0.63
2:D:378:VAL:HB	2:D:411:ARG:HG2	1.80	0.63
2:D:377:LEU:HD23	2:D:386:LEU:HD22	1.79	0.63
1:B:182:VAL:HG12	1:B:183:LYS:N	2.14	0.63
1:B:155:LEU:CD2	1:B:168:VAL:HA	2.23	0.63
1:A:80:ILE:HG21	1:A:93:VAL:HG13	1.80	0.63
2:E:466:PRO:CG	5:E:1503:GER:H71	2.26	0.63
1:A:4:ILE:HD12	1:A:51:VAL:HG11	1.81	0.62
1:A:139:TYR:N	1:A:140:PRO:HD2	2.15	0.62
2:E:421:GLU:O	2:E:451:PRO:HG3	1.99	0.62
2:E:346:GLU:HG3	2:E:347:SER:N	2.15	0.61
1:B:138:THR:OG1	1:B:141:GLN:HG3	2.00	0.61
2:E:396:SER:O	2:E:400:GLN:HG3	2.00	0.61
1:A:102:ARG:NH1	1:A:110:ILE:CD1	2.63	0.60
1:B:65:ASP:HA	1:B:68:ARG:NH1	2.07	0.60
1:B:100:GLU:HG3	2:E:327:TYR:HE1	1.66	0.60
2:E:382:ALA:HB2	2:E:502:TRP:CE2	2.36	0.60
2:E:472:ARG:HG2	2:E:498:ILE:O	2.01	0.59
1:B:80:ILE:O	1:B:112:LEU:HD12	2.01	0.59
1:A:14:VAL:O	1:A:116:LYS:HE3	2.02	0.59
1:B:102:ARG:HH12	1:B:110:ILE:HD11	1.67	0.59
1:B:51:VAL:HG21	1:B:173:ILE:HD12	1.84	0.59
1:A:155:LEU:CD1	1:A:168:VAL:HA	2.33	0.59
1:B:11:ASP:OD1	1:B:92:ASN:ND2	2.34	0.59
2:D:394:LEU:HD13	2:D:492:TRP:HB3	1.85	0.59
1:B:102:ARG:HH11	1:B:102:ARG:HA	1.68	0.59
1:A:118:ASP:OD2	1:A:160:LEU:HB3	2.02	0.58
1:A:126:ILE:O	1:A:126:ILE:HG22	2.03	0.58
1:B:80:ILE:CD1	1:B:101:VAL:HG21	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:342:ASP:HB2	2:D:348:LEU:HD23	1.85	0.58
2:D:435:LYS:O	2:D:437:VAL:HG23	2.03	0.58
1:B:44:VAL:O	1:B:50:PRO:HA	2.04	0.58
2:E:346:GLU:OE2	2:E:350:LYS:HE3	2.03	0.58
1:B:124:ASP:N	1:B:124:ASP:OD1	2.30	0.57
2:E:421:GLU:CD	2:E:422:ILE:H	2.07	0.57
2:E:376:THR:HB	2:E:413:LYS:HB3	1.85	0.57
1:B:118:ASP:OD2	1:B:158:SER:HB2	2.05	0.56
2:D:411:ARG:NH1	2:D:462:VAL:HG22	2.21	0.56
2:D:390:LEU:HD22	2:D:490:LEU:HD21	1.86	0.56
1:B:111:ILE:HD11	1:B:172:ALA:HA	1.87	0.56
1:B:183:LYS:N	1:B:183:LYS:CD	2.56	0.56
1:B:16:LYS:O	1:B:20:LEU:HD23	2.06	0.56
1:A:96:LYS:O	1:A:99:PRO:HG2	2.06	0.56
2:D:407:GLY:HA2	2:D:465:ALA:O	2.04	0.56
2:D:346:GLU:OE2	2:D:350:LYS:HE3	2.06	0.56
2:E:364:ASP:C	2:E:364:ASP:OD1	2.44	0.56
1:A:125:THR:O	1:A:129:LEU:HB2	2.06	0.55
1:A:20:LEU:CD1	1:A:57:ASP:HB2	2.35	0.55
1:A:83:SER:HB3	1:A:86:SER:HB3	1.88	0.55
1:B:22:SER:CB	1:B:159:ALA:HB1	2.37	0.55
1:B:139:TYR:HE1	1:B:143:LEU:HD22	1.70	0.55
1:B:181:PRO:O	1:B:182:VAL:HG22	2.07	0.55
1:B:40:TYR:HD2	1:B:55:LEU:HD12	1.72	0.55
2:E:343:LYS:HD2	2:E:349:ARG:HD3	1.89	0.55
2:D:337:GLU:HA	2:D:340:GLU:HG2	1.88	0.54
1:A:73:PRO:O	1:A:74:GLN:HB2	2.06	0.54
2:E:366:ASN:CG	2:E:367:VAL:N	2.59	0.54
1:B:46:VAL:CG1	1:B:174:ARG:NE	2.70	0.54
2:D:371:VAL:HG13	2:D:417:ARG:HB3	1.89	0.54
1:A:20:LEU:HD12	1:A:57:ASP:HB2	1.88	0.54
1:A:64:TYR:CZ	2:D:341:LEU:CD1	2.88	0.54
2:D:388:LEU:HD22	2:D:397:PHE:CE2	2.43	0.54
2:E:466:PRO:HG3	5:E:1503:GER:H102	1.88	0.54
2:D:396:SER:HB2	2:D:400:GLN:HE21	1.73	0.54
2:D:421:GLU:CD	2:D:422:ILE:H	2.11	0.54
2:E:468:GLY:C	2:E:470:LEU:H	2.09	0.54
2:D:482:THR:HA	2:D:487:THR:O	2.07	0.54
2:E:405:LYS:O	2:E:408:VAL:HG22	2.08	0.54
2:D:424:SER:O	2:D:483:ASP:HB2	2.07	0.54
2:E:386:LEU:N	2:E:386:LEU:HD12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HG12	1:B:37:PHE:O	2.09	0.53
1:B:98:TYR:CD1	1:B:149:ILE:HB	2.43	0.53
2:E:371:VAL:CG1	2:E:417:ARG:HB3	2.38	0.53
2:D:434:ARG:O	2:D:435:LYS:HB2	2.08	0.53
2:E:361:VAL:HG11	2:E:419:ASN:O	2.08	0.53
2:E:490:LEU:HG	2:E:491:SER:H	1.73	0.53
1:B:166:LYS:HE3	1:B:170:ASP:OD2	2.09	0.53
1:B:53:LEU:CD2	1:B:55:LEU:HD21	2.39	0.53
1:B:46:VAL:CG1	1:B:174:ARG:HE	2.23	0.52
2:E:428:TYR:HE1	2:E:479:SER:HB3	1.74	0.52
1:A:17:THR:HG23	1:A:37:PHE:HB2	1.92	0.52
2:E:377:LEU:HD13	5:E:1503:GER:H203	1.92	0.52
1:A:132:LYS:O	1:A:133:LYS:HB2	2.10	0.52
1:B:102:ARG:NH1	1:B:110:ILE:CD1	2.73	0.52
2:E:334:SER:HA	2:E:421:GLU:OE2	2.10	0.52
2:E:421:GLU:OE1	2:E:422:ILE:N	2.38	0.52
1:B:8:VAL:HG21	1:B:20:LEU:HD21	1.92	0.52
1:B:8:VAL:HG22	1:B:79:LEU:HD12	1.92	0.52
1:B:35:THR:O	6:B:2001:HOH:O	2.19	0.51
1:B:53:LEU:HD13	1:B:173:ILE:CD1	2.37	0.51
2:E:378:VAL:HG21	2:E:459:LEU:HD21	1.91	0.51
1:B:11:ASP:CG	1:B:92:ASN:HD22	2.14	0.51
2:E:346:GLU:CD	2:E:350:LYS:HE3	2.30	0.51
1:A:98:TYR:N	1:A:99:PRO:HD2	2.25	0.51
2:E:411:ARG:HD3	2:E:459:LEU:HB3	1.93	0.51
2:E:416:PHE:N	2:E:416:PHE:CD1	2.78	0.51
2:E:423:VAL:O	2:E:448:SER:HA	2.11	0.51
1:A:129:LEU:CD2	1:A:134:LEU:HB3	2.41	0.50
2:E:346:GLU:HA	2:E:349:ARG:HH12	1.75	0.50
1:A:182:VAL:HG12	1:A:183:LYS:N	2.26	0.50
1:B:25:THR:O	1:B:26:ASN:HB2	2.11	0.50
1:A:48:GLY:O	1:A:49:LYS:HG2	2.11	0.50
1:B:163:ARG:HG2	1:B:163:ARG:O	2.10	0.50
2:D:334:SER:HG	2:D:337:GLU:HG3	1.75	0.50
2:E:407:GLY:HA2	2:E:465:ALA:O	2.11	0.50
1:B:173:ILE:O	1:B:177:LEU:HB2	2.12	0.50
2:E:472:ARG:NH1	2:E:500:LYS:CD	2.62	0.50
1:B:181:PRO:O	1:B:182:VAL:CG2	2.59	0.50
2:E:346:GLU:HA	2:E:349:ARG:NH1	2.26	0.50
1:B:79:LEU:HD23	1:B:111:ILE:HB	1.94	0.50
1:B:103:HIS:O	2:E:445:MET:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HG11	1:B:72:TYR:OH	2.12	0.50
2:E:366:ASN:C	2:E:366:ASN:ND2	2.65	0.50
1:B:122:ASP:O	1:B:126:ILE:HG13	2.12	0.49
1:B:68:ARG:NH1	1:B:68:ARG:HB3	2.27	0.49
1:B:76:ASP:O	1:B:109:PRO:HD2	2.12	0.49
2:D:468:GLY:C	2:D:470:LEU:H	2.11	0.49
2:E:366:ASN:O	2:E:367:VAL:C	2.51	0.49
1:B:66:ARG:NH1	2:E:332:GLN:OE1	2.45	0.49
1:B:53:LEU:HD21	1:B:55:LEU:HD21	1.94	0.49
1:A:142:GLY:HA3	1:A:154:TYR:CZ	2.47	0.49
1:B:51:VAL:HG21	1:B:173:ILE:CD1	2.42	0.49
2:E:471:ALA:HB1	2:E:475:TYR:OH	2.13	0.49
1:B:100:GLU:HG3	2:E:327:TYR:CE1	2.45	0.49
1:B:119:LEU:HD21	3:B:1190:GDP:N2	2.27	0.49
2:D:342:ASP:CB	2:D:348:LEU:HD23	2.43	0.48
2:E:499:LYS:NZ	6:E:2005:HOH:O	2.46	0.48
2:E:335:ILE:HD11	2:E:451:PRO:CD	2.43	0.48
1:A:87:PRO:CG	1:A:134:LEU:HD12	2.43	0.48
1:A:67:LEU:HD23	1:A:68:ARG:N	2.29	0.48
1:A:7:VAL:HG22	1:A:75:THR:HG21	1.93	0.48
1:B:138:THR:H	1:B:141:GLN:NE2	2.11	0.48
2:D:371:VAL:HG13	2:D:371:VAL:O	2.13	0.48
2:E:428:TYR:CE1	2:E:479:SER:HB3	2.49	0.48
2:E:466:PRO:HG3	5:E:1503:GER:C7	2.31	0.48
1:B:182:VAL:CG2	1:B:185:ARG:HH12	2.14	0.48
2:D:377:LEU:HD13	5:D:1502:GER:H161	1.95	0.48
2:E:432:THR:HB	2:E:440:ASP:HB3	1.95	0.48
1:B:175:ALA:O	1:B:179:PRO:CG	2.62	0.48
2:E:335:ILE:O	2:E:338:ILE:HB	2.14	0.47
1:A:90:PHE:CE1	1:A:145:MET:HG3	2.48	0.47
1:A:175:ALA:O	1:A:179:PRO:HG3	2.14	0.47
1:B:83:SER:HB3	1:B:86:SER:HB3	1.95	0.47
2:E:411:ARG:HG2	2:E:459:LEU:HD22	1.97	0.47
2:E:337:GLU:HA	2:E:340:GLU:HG2	1.97	0.47
2:E:468:GLY:C	2:E:470:LEU:N	2.67	0.47
1:B:28:PHE:HA	1:B:29:PRO:HD3	1.80	0.47
2:D:409:GLU:HA	2:D:463:GLU:O	2.15	0.47
2:E:482:THR:HA	2:E:487:THR:O	2.14	0.47
1:A:123:LYS:CE	1:A:123:LYS:HA	2.38	0.47
1:B:46:VAL:HG13	1:B:174:ARG:HE	1.79	0.47
1:A:179:PRO:HB2	1:A:180:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:ASP:C	2:D:391:THR:H	2.19	0.46
1:A:179:PRO:CB	1:A:180:PRO:HD2	2.45	0.46
1:B:44:VAL:HG12	1:B:45:MET:N	2.30	0.46
1:A:67:LEU:HD21	2:D:351:TYR:CE2	2.50	0.46
1:B:102:ARG:HH12	1:B:110:ILE:CD1	2.28	0.46
1:B:40:TYR:CG	1:B:41:SER:N	2.83	0.46
1:B:139:TYR:N	1:B:140:PRO:CD	2.78	0.46
2:D:371:VAL:CG1	2:D:417:ARG:HB3	2.46	0.46
1:A:69:PRO:HA	1:A:72:TYR:CE2	2.51	0.46
2:D:423:VAL:O	2:D:448:SER:HA	2.16	0.46
1:A:90:PHE:CZ	1:A:145:MET:CG	2.98	0.46
2:D:434:ARG:HB2	2:D:475:TYR:CD2	2.51	0.46
1:B:35:THR:HG21	2:E:348:LEU:HD21	1.97	0.46
1:B:41:SER:CA	1:B:53:LEU:O	2.55	0.46
1:B:173:ILE:CG2	1:B:177:LEU:HD12	2.45	0.46
1:B:11:ASP:OD2	1:B:89:SER:HA	2.16	0.45
2:D:411:ARG:CG	2:D:459:LEU:HD22	2.44	0.45
1:A:44:VAL:HG21	1:A:173:ILE:CD1	2.46	0.45
1:B:40:TYR:CD2	1:B:55:LEU:HD12	2.49	0.45
2:D:370:VAL:HG12	2:D:371:VAL:N	2.31	0.45
2:E:411:ARG:CD	2:E:459:LEU:HD22	2.46	0.45
1:B:37:PHE:CE2	1:B:40:TYR:HB2	2.51	0.45
2:E:349:ARG:HH11	2:E:349:ARG:HG3	1.82	0.45
1:A:123:LYS:O	1:A:127:GLU:HG3	2.16	0.45
1:B:18:CYS:SG	1:B:28:PHE:HE1	2.40	0.45
1:B:96:LYS:C	1:B:99:PRO:HD2	2.36	0.45
2:D:377:LEU:HB3	2:D:386:LEU:HB3	1.99	0.45
2:D:496:LEU:HG	2:D:497:THR:N	2.32	0.45
1:B:182:VAL:CG1	1:B:183:LYS:N	2.79	0.45
1:B:68:ARG:HB3	1:B:68:ARG:HH11	1.80	0.45
2:D:323:HIS:ND1	2:D:323:HIS:O	2.49	0.45
2:D:376:THR:HB	2:D:413:LYS:HD3	1.99	0.45
2:E:333:LYS:HB2	2:E:333:LYS:HE3	1.74	0.45
1:A:67:LEU:C	1:A:67:LEU:HD23	2.37	0.45
1:A:67:LEU:HD12	2:D:338:ILE:HG21	2.00	0.44
1:B:97:TRP:O	1:B:101:VAL:HG23	2.17	0.44
1:B:126:ILE:HG22	1:B:126:ILE:O	2.17	0.44
1:A:10:GLY:O	1:A:16:LYS:HE2	2.18	0.44
1:B:117:LEU:HD12	1:B:120:ARG:HD3	1.99	0.44
1:A:178:CYS:N	1:A:179:PRO:CD	2.80	0.44
2:E:392:GLY:O	2:E:394:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASP:CG	1:A:174:ARG:HH11	2.21	0.44
1:A:18:CYS:SG	1:A:33:ILE:HD13	2.57	0.44
1:B:166:LYS:HG3	1:B:167:THR:N	2.32	0.44
1:B:111:ILE:CD1	1:B:172:ALA:HA	2.46	0.44
2:D:390:LEU:HD13	2:D:490:LEU:CD2	2.48	0.44
1:A:14:VAL:CG2	1:A:16:LYS:HG3	2.48	0.44
2:E:361:VAL:HG11	2:E:451:PRO:HB3	2.00	0.44
2:E:433:TYR:CE1	2:E:478:LYS:HE2	2.53	0.44
1:B:11:ASP:O	1:B:14:VAL:HG22	2.17	0.44
2:D:432:THR:HG21	5:D:1502:GER:H93	2.00	0.44
1:A:98:TYR:CD1	1:A:149:ILE:HB	2.52	0.43
1:B:142:GLY:HA3	1:B:154:TYR:CZ	2.52	0.43
2:D:341:LEU:HD23	2:D:341:LEU:HA	1.77	0.43
2:E:345:ASP:OD1	2:E:347:SER:HB3	2.18	0.43
1:B:152:VAL:O	1:B:153:LYS:HD3	2.17	0.43
2:D:367:VAL:HA	2:D:368:PRO:HD3	1.85	0.43
2:D:405:LYS:HE2	2:D:408:VAL:CG1	2.48	0.43
1:A:102:ARG:HH11	1:A:102:ARG:CB	2.30	0.43
2:D:329:PRO:HA	2:D:330:PRO:HD3	1.74	0.43
2:E:387:GLU:CG	2:E:388:LEU:N	2.80	0.43
2:E:377:LEU:HD11	2:E:410:TYR:CD2	2.54	0.43
1:B:116:LYS:HB3	1:B:119:LEU:HD12	2.01	0.43
2:E:434:ARG:C	2:E:435:LYS:HG3	2.39	0.43
1:A:87:PRO:HG2	1:A:134:LEU:CD1	2.48	0.43
1:B:154:TYR:O	1:B:155:LEU:HD12	2.19	0.43
2:E:451:PRO:O	2:E:452:ARG:HB3	2.18	0.43
2:E:479:SER:HB2	2:E:492:TRP:CZ3	2.54	0.43
1:B:28:PHE:CE2	1:B:29:PRO:O	2.72	0.43
2:D:426:MET:HA	2:D:483:ASP:HB3	2.00	0.43
1:B:181:PRO:C	1:B:182:VAL:CG2	2.86	0.43
1:B:37:PHE:HB3	1:B:57:ASP:HB2	1.99	0.43
2:D:414:ILE:HG21	2:D:481:PHE:HE2	1.84	0.43
1:B:80:ILE:HD11	1:B:101:VAL:HG21	2.00	0.43
1:B:131:GLU:HG2	1:B:131:GLU:O	2.18	0.42
2:D:466:PRO:HG3	5:D:1502:GER:H71	2.00	0.42
2:E:494:TRP:CD1	2:E:494:TRP:N	2.86	0.42
2:D:390:LEU:HD13	2:D:490:LEU:HD23	2.00	0.42
2:D:468:GLY:C	2:D:470:LEU:N	2.68	0.42
2:E:394:LEU:HD22	2:E:397:PHE:CE1	2.54	0.42
2:E:434:ARG:O	2:E:435:LYS:CB	2.67	0.42
1:B:167:THR:HA	1:B:170:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:434:ARG:O	2:E:435:LYS:HB2	2.20	0.42
1:A:11:ASP:O	1:A:14:VAL:HG13	2.20	0.42
1:B:18:CYS:HG	1:B:28:PHE:HE1	1.65	0.42
2:E:475:TYR:HE1	2:E:498:ILE:HG12	1.84	0.42
1:B:119:LEU:HD21	3:B:1190:GDP:HN21	1.83	0.42
2:E:371:VAL:HG13	2:E:371:VAL:O	2.19	0.42
2:D:377:LEU:HD11	2:D:410:TYR:CD2	2.55	0.41
1:A:62:GLU:O	1:A:62:GLU:HG2	2.19	0.41
1:B:129:LEU:CD1	1:B:134:LEU:HB3	2.50	0.41
1:B:138:THR:OG1	1:B:140:PRO:HG2	2.20	0.41
1:B:181:PRO:C	1:B:182:VAL:HG23	2.40	0.41
2:D:488:ASP:OD1	2:D:488:ASP:C	2.59	0.41
1:A:12:GLY:O	1:A:13:ALA:HB3	2.21	0.41
1:A:62:GLU:HA	1:A:65:ASP:OD1	2.19	0.41
1:B:73:PRO:O	1:B:74:GLN:HB2	2.21	0.41
1:B:65:ASP:CG	1:B:96:LYS:HZ1	2.24	0.41
2:D:372:VAL:HB	2:D:490:LEU:HD22	2.03	0.41
2:E:460:THR:HB	2:E:461:PRO:CD	2.51	0.41
1:B:182:VAL:HG12	1:B:183:LYS:H	1.81	0.41
1:B:24:THR:CG2	1:B:40:TYR:CE2	3.03	0.41
2:E:341:LEU:HD23	2:E:341:LEU:HA	1.85	0.41
2:E:361:VAL:HG11	2:E:451:PRO:CB	2.50	0.41
1:B:31:GLU:HG3	1:B:32:TYR:N	2.34	0.41
2:D:416:PHE:N	2:D:416:PHE:CD1	2.88	0.41
2:E:446:VAL:HG13	2:E:458:PHE:CD2	2.56	0.41
1:A:126:ILE:HG22	1:A:130:LYS:HD2	2.03	0.41
2:E:434:ARG:HH12	2:E:473:GLY:CA	2.15	0.41
2:E:435:LYS:O	2:E:437:VAL:HG23	2.20	0.41
1:A:177:LEU:O	1:A:178:CYS:CB	2.69	0.40
1:A:5:LYS:HE3	1:A:56:TRP:NE1	2.35	0.40
1:B:113:VAL:HA	1:B:155:LEU:O	2.21	0.40
1:B:138:THR:HB	1:B:140:PRO:HD2	2.03	0.40
1:B:74:GLN:CA	1:B:74:GLN:NE2	2.80	0.40
1:A:139:TYR:N	1:A:140:PRO:CD	2.84	0.40
1:B:24:THR:HG22	1:B:40:TYR:CE2	2.57	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	187/192 (97%)	173 (92%)	11 (6%)	3 (2%)	9	24
1	B	187/192 (97%)	164 (88%)	18 (10%)	5 (3%)	5	12
2	D	182/204 (89%)	148 (81%)	27 (15%)	7 (4%)	3	7
2	E	178/204 (87%)	147 (83%)	23 (13%)	8 (4%)	2	5
All	All	734/792 (93%)	632 (86%)	79 (11%)	23 (3%)	4	9

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	CYS
2	E	362	SER
2	E	366	ASN
2	D	314	ILE
2	D	383	PRO
2	D	390	LEU
2	E	341	LEU
2	E	365	PRO
1	B	39	ASN
1	B	41	SER
2	D	341	LEU
2	E	364	ASP
1	A	126	ILE
1	A	178	CYS
2	D	440	ASP
1	A	188	LYS
2	E	359	VAL
1	B	126	ILE
2	D	326	ASN
2	D	385	PRO
2	E	367	VAL
2	E	435	LYS
1	B	30	GLY

### 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	160/168 (95%)	144 (90%)	16 (10%)	7	18
1	B	159/168 (95%)	147 (92%)	12 (8%)	13	31
2	D	152/180 (84%)	139 (91%)	13 (9%)	10	24
2	E	159/180 (88%)	148 (93%)	11 (7%)	15	35
All	All	630/696 (90%)	578 (92%)	52 (8%)	11	25

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	31	GLU
1	A	38	ASP
1	A	39	ASN
1	A	45	MET
1	A	61	GLN
1	A	67	LEU
1	A	70	LEU
1	A	102	ARG
1	A	120	ARG
1	A	123	LYS
1	A	129	LEU
1	A	134	LEU
1	A	158	SER
1	A	166	LYS
1	A	189	CYS
1	B	38	ASP
1	B	39	ASN
1	B	63	ASP
1	B	102	ARG
1	B	107	ASN
1	B	124	ASP
1	B	134	LEU
1	B	163	ARG

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Mol	Chain	Res	Type
1	B	166	LYS
1	B	183	LYS
1	B	186	LYS
1	B	189	CYS
2	D	320	GLU
2	D	326	ASN
2	D	336	GLN
2	D	338	ILE
2	D	341	LEU
2	D	343	LYS
2	D	348	LEU
2	D	358	ARG
2	D	366	ASN
2	D	386	LEU
2	D	389	ASP
2	D	413	LYS
2	D	501	ASP
2	E	323	HIS
2	E	336	GLN
2	E	346	GLU
2	E	348	LEU
2	E	364	ASP
2	E	366	ASN
2	E	409	GLU
2	E	416	PHE
2	E	423	VAL
2	E	494	TRP
2	E	502	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	39	ASN
1	B	39	ASN
1	B	61	GLN
1	B	74	GLN
1	B	141	GLN
1	B	162	GLN
2	D	326	ASN
2	D	366	ASN
2	D	400	GLN

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Mol	Chain	Res	Type
2	D	430	GLN
2	E	339	GLN
2	E	366	ASN
2	E	430	GLN

### 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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
3	GDP	B	1190	4	24,30,30	2.91	11 (45%)	31,47,47	3.42	9 (29%)
5	GER	D	1502	-	19,19,19	1.49	4 (21%)	22,22,22	3.01	12 (54%)
3	GDP	A	1190	4	24,30,30	2.80	9 (37%)	31,47,47	3.49	8 (25%)
5	GER	E	1503	-	19,19,19	1.51	4 (21%)	22,22,22	2.97	12 (54%)

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
3	GDP	B	1190	4	-	3/12/32/32	0/3/3/3
5	GER	D	1502	-	-	7/20/20/20	-
3	GDP	A	1190	4	-	3/12/32/32	0/3/3/3
5	GER	E	1503	-	-	5/20/20/20	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1190	GDP	C2-N1	9.07	1.51	1.35
3	A	1190	GDP	C2-N1	8.40	1.50	1.35
3	A	1190	GDP	O4'-C1'	6.25	1.49	1.41
3	B	1190	GDP	O4'-C1'	6.01	1.49	1.41
3	A	1190	GDP	PB-O2B	-4.29	1.38	1.54
3	B	1190	GDP	PB-O2B	-4.00	1.39	1.54
3	B	1190	GDP	O6-C6	3.91	1.34	1.24
3	A	1190	GDP	O6-C6	3.84	1.34	1.24
3	B	1190	GDP	C8-N7	3.76	1.41	1.34
3	A	1190	GDP	C8-N7	3.17	1.40	1.34
5	D	1502	GER	C10-C8	2.79	1.57	1.51
5	E	1503	GER	C10-C8	2.74	1.57	1.51
5	E	1503	GER	C12-C13	2.42	1.38	1.33
3	A	1190	GDP	C5-C4	2.40	1.47	1.40
5	D	1502	GER	C7-C8	2.21	1.38	1.33
3	B	1190	GDP	C6-N1	2.21	1.36	1.33
3	B	1190	GDP	O4'-C4'	2.20	1.49	1.45
5	E	1503	GER	C7-C8	2.16	1.38	1.33
3	A	1190	GDP	PB-O3B	2.15	1.63	1.54
3	B	1190	GDP	C3'-C4'	2.15	1.58	1.53
3	B	1190	GDP	O3'-C3'	2.14	1.48	1.43
3	A	1190	GDP	O3'-C3'	2.10	1.47	1.43
3	A	1190	GDP	O4'-C4'	2.09	1.49	1.45
5	E	1503	GER	C5-C3	2.09	1.55	1.51
3	B	1190	GDP	PB-O3B	2.07	1.62	1.54
5	D	1502	GER	C5-C3	2.05	1.55	1.51
5	D	1502	GER	C12-C13	2.04	1.37	1.33
3	B	1190	GDP	C5-C4	2.01	1.46	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1190	GDP	C6-C5-C4	-12.23	109.12	120.80
3	B	1190	GDP	C6-C5-C4	-11.57	109.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1190	GDP	N2-C2-N3	8.74	132.03	117.79
3	B	1190	GDP	N2-C2-N3	8.35	131.41	117.79
5	E	1503	GER	C9-C8-C10	7.18	127.35	115.27
5	D	1502	GER	C9-C8-C10	7.11	127.23	115.27
5	D	1502	GER	C20-C18-C19	6.21	128.33	114.60
3	A	1190	GDP	N2-C2-N1	-6.20	107.61	117.25
5	E	1503	GER	C20-C18-C19	5.98	127.82	114.60
3	B	1190	GDP	N3-C2-N1	-5.64	119.70	127.22
3	B	1190	GDP	N2-C2-N1	-5.38	108.89	117.25
3	B	1190	GDP	C4-C5-N7	-5.30	103.88	109.40
3	A	1190	GDP	C4-C5-N7	-5.25	103.93	109.40
3	A	1190	GDP	N3-C2-N1	-5.14	120.36	127.22
3	B	1190	GDP	C2-N3-C4	4.70	120.72	115.36
5	D	1502	GER	C4-C3-C5	4.22	122.37	115.27
5	E	1503	GER	C4-C3-C5	4.22	122.37	115.27
3	A	1190	GDP	C2-N3-C4	4.03	119.96	115.36
5	D	1502	GER	C6-C5-C3	3.58	124.75	112.98
5	D	1502	GER	C14-C13-C15	3.44	121.06	115.27
3	B	1190	GDP	C2'-C3'-C4'	3.43	109.31	102.64
5	E	1503	GER	C6-C5-C3	3.37	124.06	112.98
5	E	1503	GER	C14-C13-C15	3.33	120.87	115.27
5	E	1503	GER	C16-C15-C13	3.24	123.62	112.98
5	D	1502	GER	C20-C18-C17	-3.13	113.60	122.65
5	D	1502	GER	C16-C15-C13	3.10	123.16	112.98
5	E	1503	GER	C20-C18-C17	-3.05	113.85	122.65
3	A	1190	GDP	C2'-C3'-C4'	3.01	108.48	102.64
5	D	1502	GER	C11-C10-C8	2.97	122.73	112.98
5	D	1502	GER	C10-C8-C7	-2.90	115.24	121.12
5	E	1503	GER	C4-C3-C2	-2.84	118.19	123.81
5	D	1502	GER	C4-C3-C2	-2.83	118.20	123.81
5	E	1503	GER	C10-C8-C7	-2.83	115.40	121.12
5	E	1503	GER	C11-C10-C8	2.64	121.66	112.98
3	B	1190	GDP	C3'-C2'-C1'	2.54	104.80	100.98
5	E	1503	GER	C9-C8-C7	-2.50	117.25	123.68
5	D	1502	GER	C9-C8-C7	-2.40	117.53	123.68
3	A	1190	GDP	O2'-C2'-C3'	2.39	119.56	111.82
3	B	1190	GDP	O2'-C2'-C3'	2.36	119.45	111.82
5	D	1502	GER	C6-C7-C8	-2.19	122.39	127.66
5	E	1503	GER	C6-C7-C8	-2.12	122.55	127.66

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1190	GDP	PA-O3A-PB-O2B
3	B	1190	GDP	PA-O3A-PB-O2B
5	D	1502	GER	C11-C10-C8-C9
5	D	1502	GER	C14-C13-C15-C16
5	D	1502	GER	C11-C10-C8-C7
5	D	1502	GER	C12-C13-C15-C16
5	D	1502	GER	C8-C10-C11-C12
5	E	1503	GER	C4-C3-C5-C6
5	E	1503	GER	C2-C3-C5-C6
5	E	1503	GER	C3-C5-C6-C7
5	D	1502	GER	C3-C5-C6-C7
3	A	1190	GDP	PA-O3A-PB-O1B
3	B	1190	GDP	PA-O3A-PB-O1B
5	E	1503	GER	C14-C13-C15-C16
3	A	1190	GDP	PA-O3A-PB-O3B
3	B	1190	GDP	PA-O3A-PB-O3B
5	E	1503	GER	C10-C11-C12-C13
5	D	1502	GER	C10-C11-C12-C13

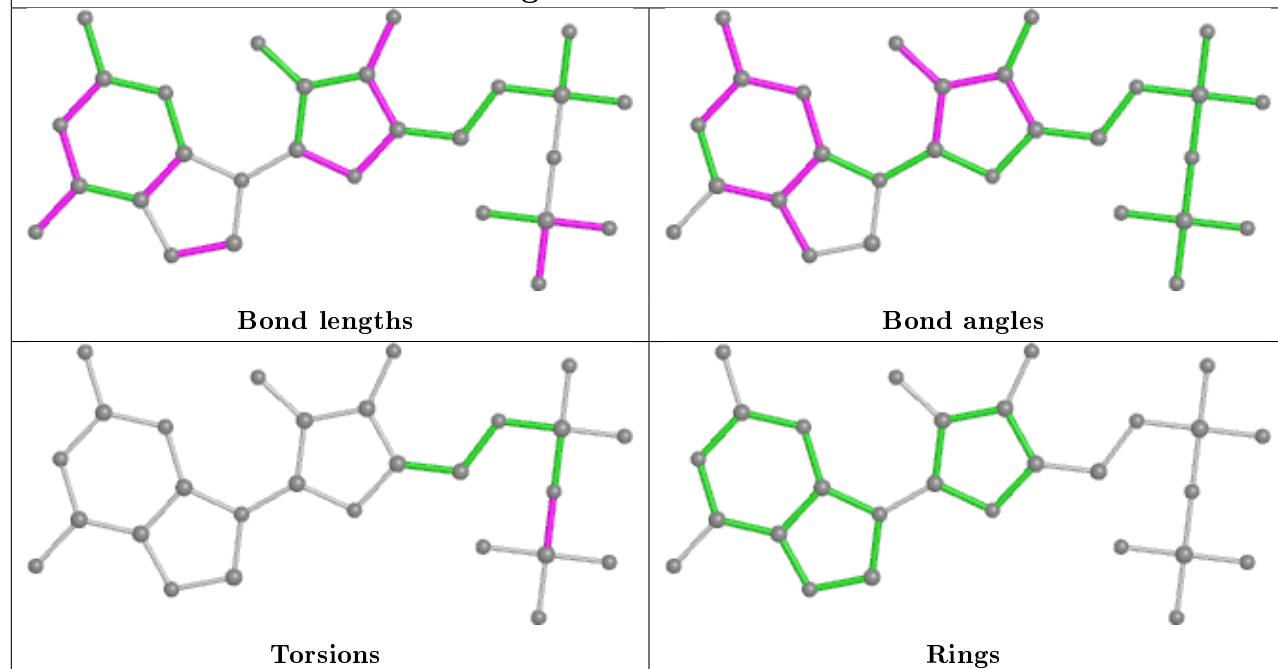
There are no ring outliers.

3 monomers are involved in 13 short contacts:

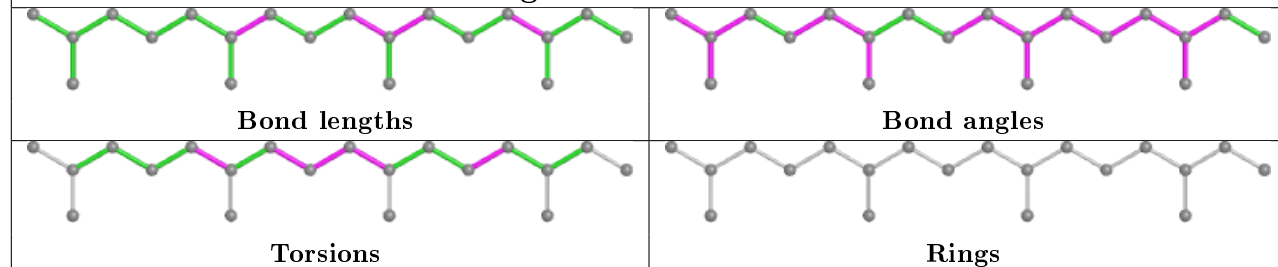
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1190	GDP	2	0
5	D	1502	GER	5	0
5	E	1503	GER	6	0

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.

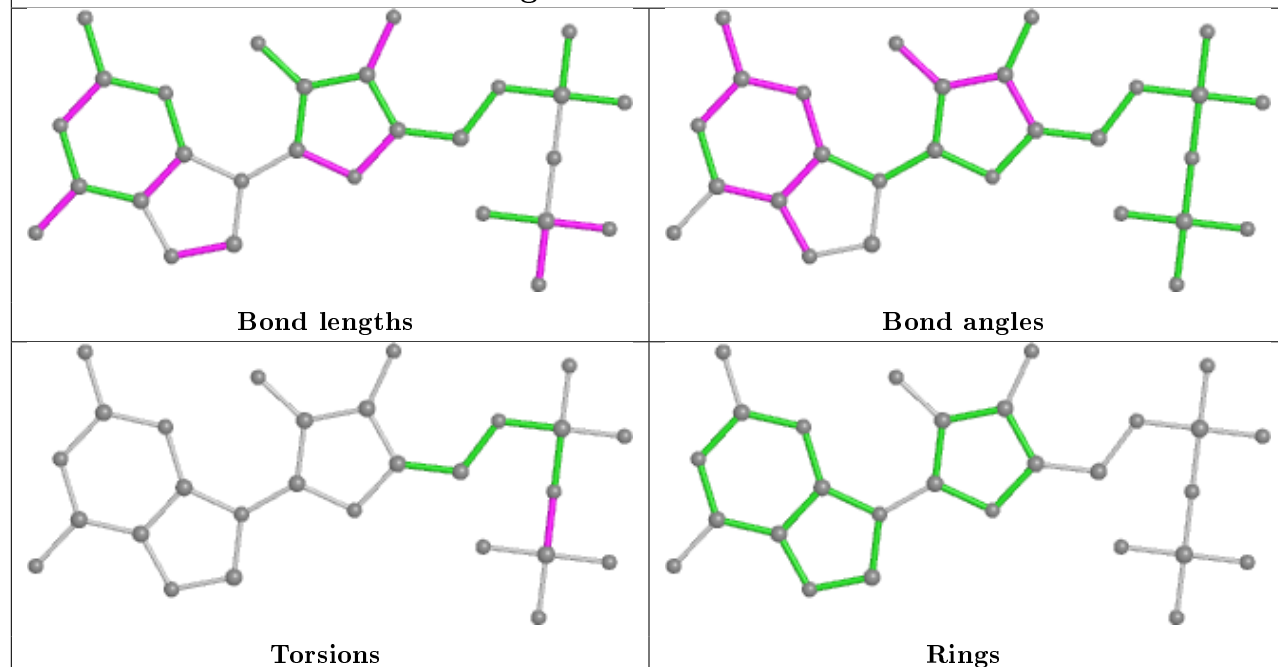
## Ligand GDP B 1190

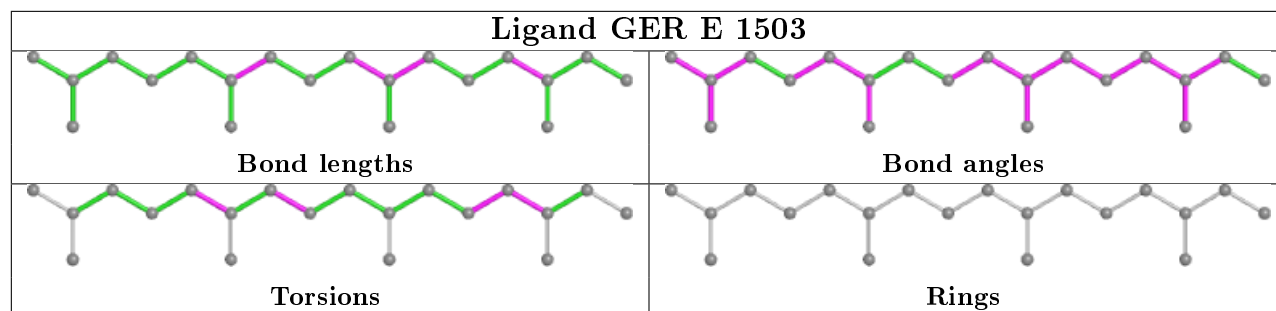


## Ligand GER D 1502



## Ligand GDP A 1190





## 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	189/192 (98%)	-0.03	11 (5%) 23 22	4, 31, 98, 132	0
1	B	189/192 (98%)	0.29	14 (7%) 14 12	11, 46, 113, 132	0
2	D	186/204 (91%)	0.47	18 (9%) 7 6	24, 67, 119, 132	0
2	E	180/204 (88%)	0.45	15 (8%) 11 9	21, 68, 110, 132	0
All	All	744/792 (93%)	0.29	58 (7%) 13 11	4, 52, 115, 132	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	CYS	7.0
2	E	359	VAL	6.3
1	B	181	PRO	6.2
2	E	367	VAL	6.1
1	A	189	CYS	6.1
1	B	182	VAL	5.4
1	B	185	ARG	5.2
2	D	383	PRO	5.0
2	D	367	VAL	4.8
1	B	31	GLU	4.7
1	A	182	VAL	4.4
2	D	396	SER	4.3
2	E	453	ALA	4.2
1	A	183	LYS	4.2
2	D	314	ILE	4.1
1	A	31	GLU	3.9
1	A	186	LYS	3.5
2	E	365	PRO	3.5
1	B	184	LYS	3.2
1	B	46	VAL	3.1
1	B	178	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	439	ILE	3.1
2	D	469	MET	3.1
2	D	319	GLU	3.1
2	D	368	PRO	3.1
2	E	469	MET	3.1
2	D	475	TYR	3.0
2	E	468	GLY	3.0
2	D	398	LYS	2.9
1	A	185	ARG	2.9
2	E	364	ASP	2.9
1	A	178	CYS	2.8
1	B	124	ASP	2.7
1	B	127	GLU	2.6
1	B	183	LYS	2.6
1	A	49	LYS	2.6
1	A	125	THR	2.5
2	E	441	LYS	2.5
2	E	435	LYS	2.4
2	D	385	PRO	2.4
2	E	344	ASP	2.3
2	D	455	GLU	2.3
2	D	317	GLU	2.3
2	E	437	VAL	2.3
2	E	366	ASN	2.3
2	D	366	ASN	2.3
1	A	188	LYS	2.3
2	D	437	VAL	2.2
2	D	434	ARG	2.2
2	E	434	ARG	2.2
2	D	310	GLN	2.2
2	E	502	TRP	2.2
1	A	184	LYS	2.2
2	E	454	GLU	2.1
1	B	186	LYS	2.1
1	B	126	ILE	2.1
1	B	131	GLU	2.1
2	D	472	ARG	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 ⓘ

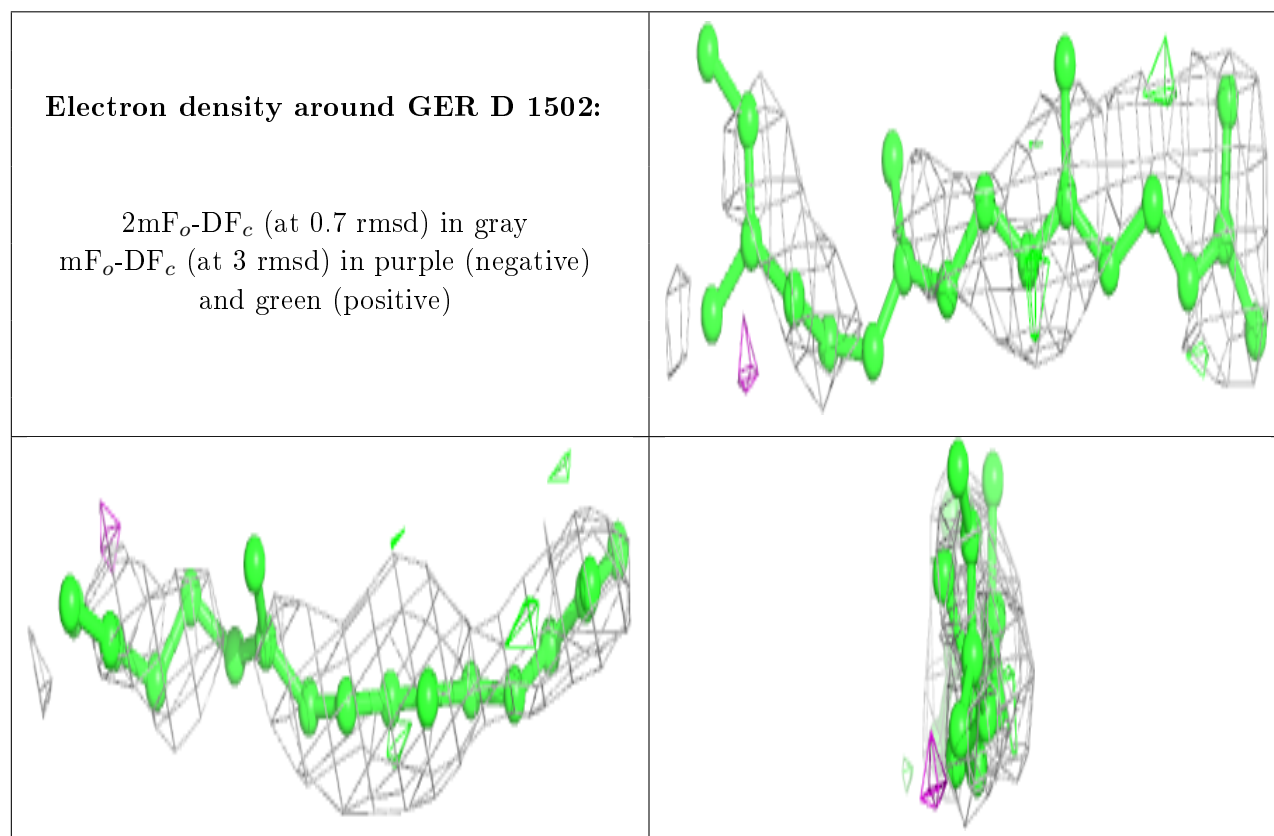
There are no carbohydrates in this entry.

### 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, 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.

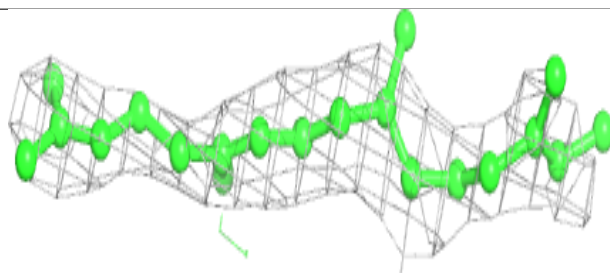
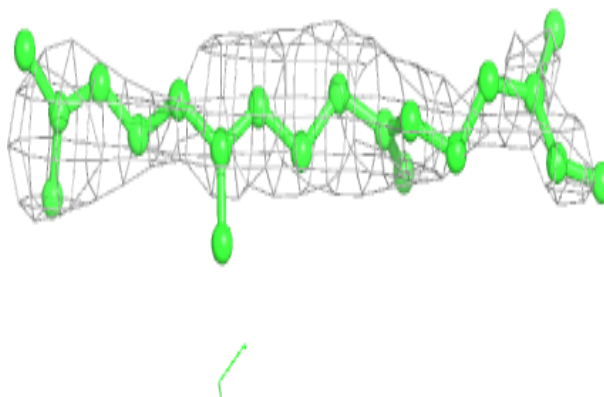
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GER	D	1502	20/20	0.56	0.49	78,78,78,78	0
5	GER	E	1503	20/20	0.71	0.33	78,78,78,78	0
4	MG	B	1191	1/1	0.94	0.57	48,48,48,48	0
3	GDP	B	1190	28/28	0.94	0.14	48,48,48,48	0
4	MG	A	1191	1/1	0.97	0.17	48,48,48,48	0
3	GDP	A	1190	28/28	0.98	0.15	38,38,38,38	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.

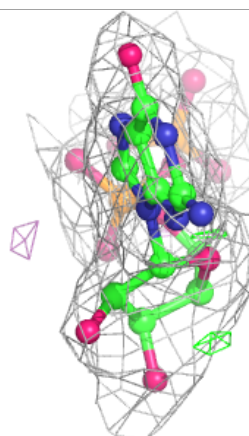
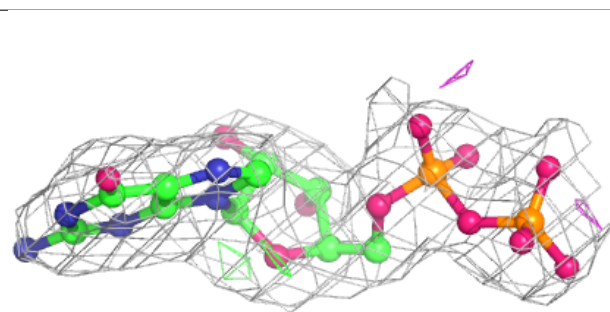
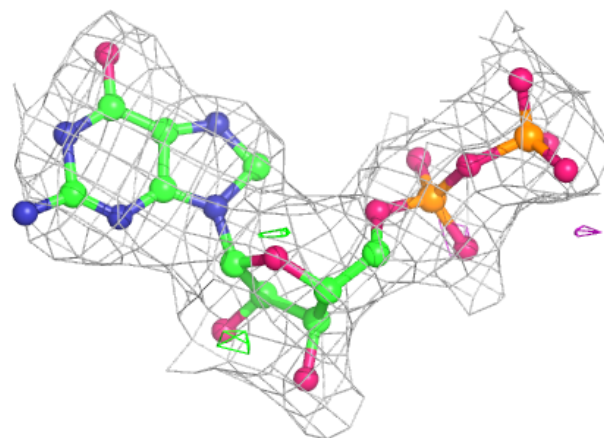


**Electron density around GER E 1503:**

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

**Electron density around GDP B 1190:**

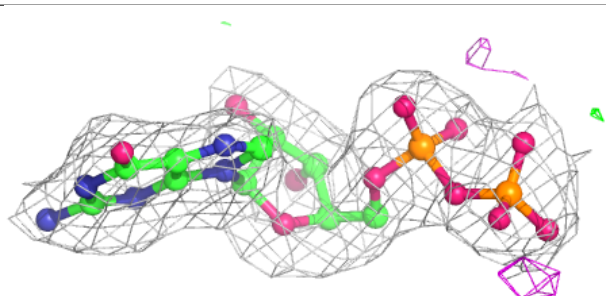
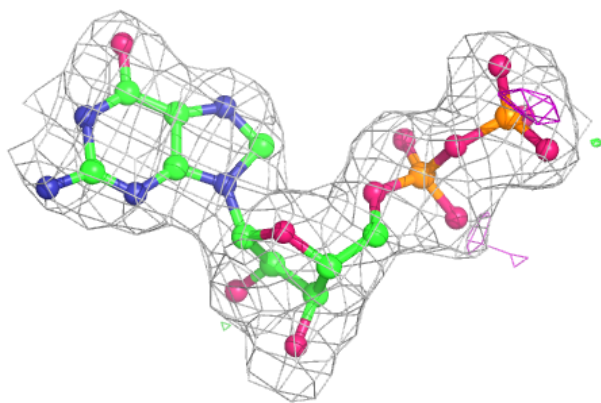
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around GDP A 1190:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.