



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:19 PM UTC

PDB ID : 1HH4 / pdb_00001hh4
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

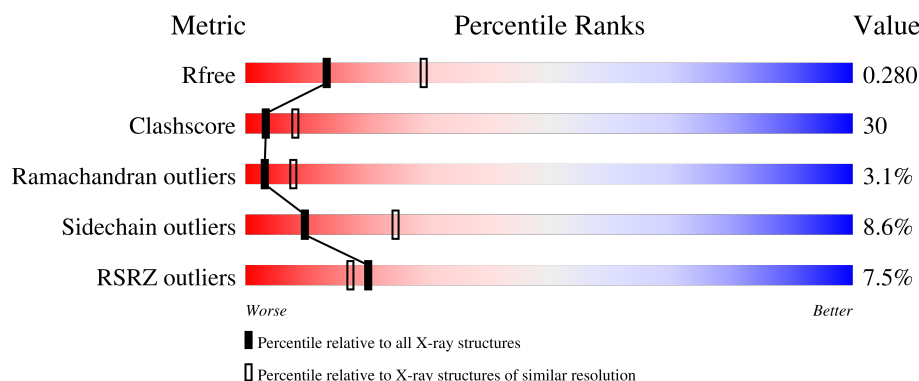
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	192	
1	B	192	
2	D	204	
2	E	204	

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			

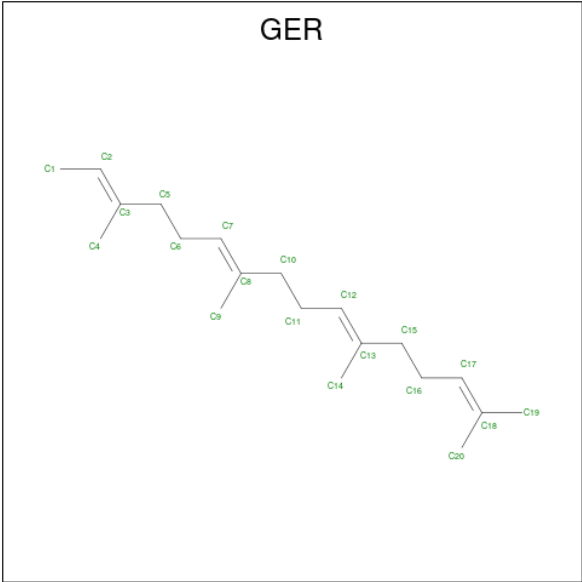
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

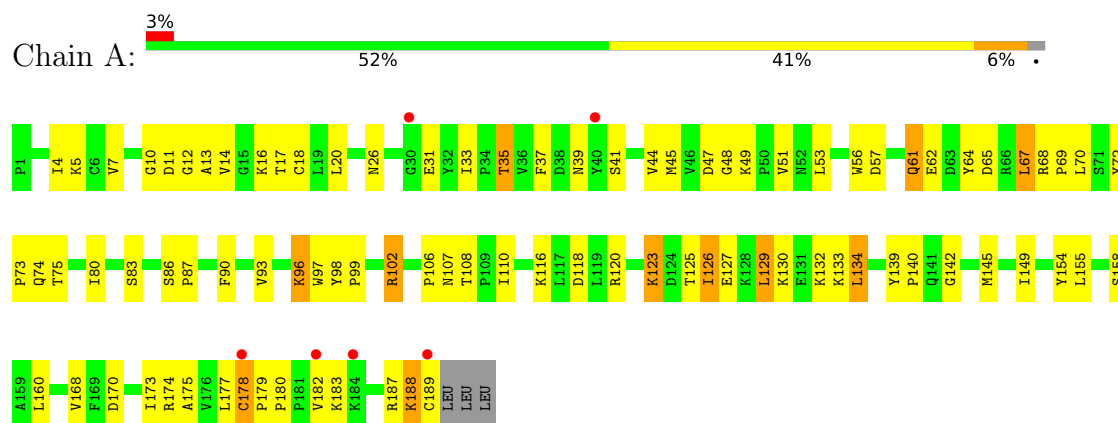
- Molecule 6 is water.

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

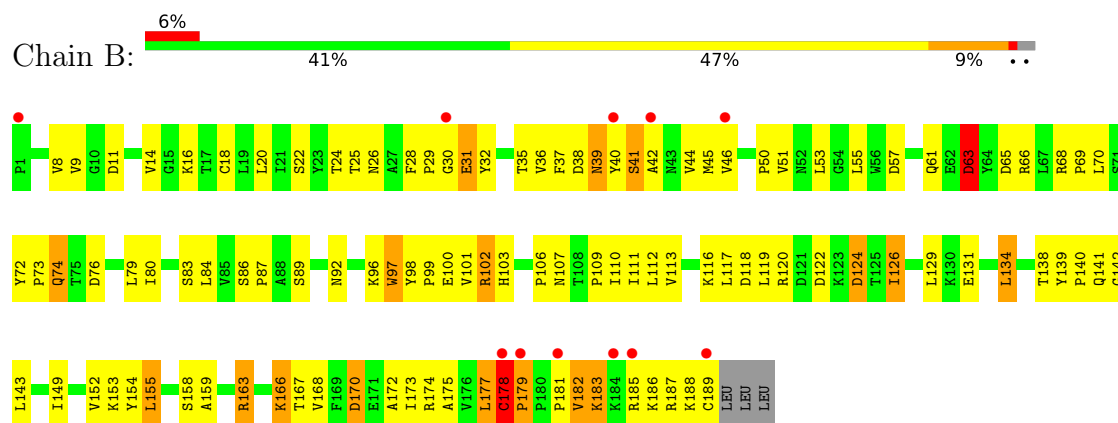
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

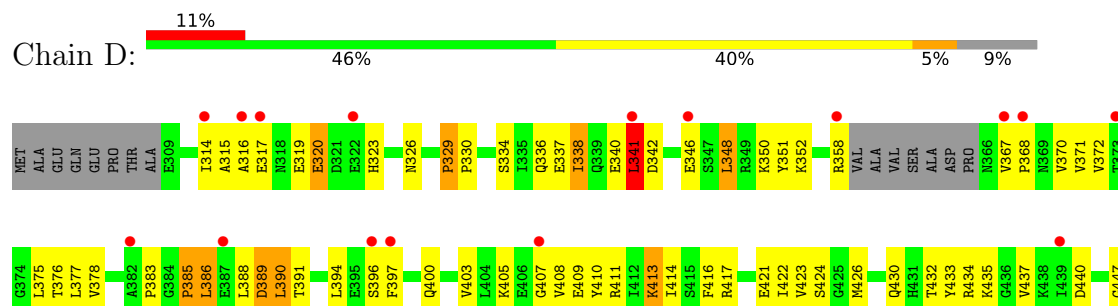
• Molecule 1: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1

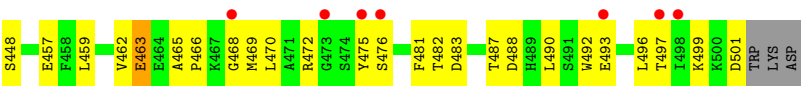


• Molecule 1: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1

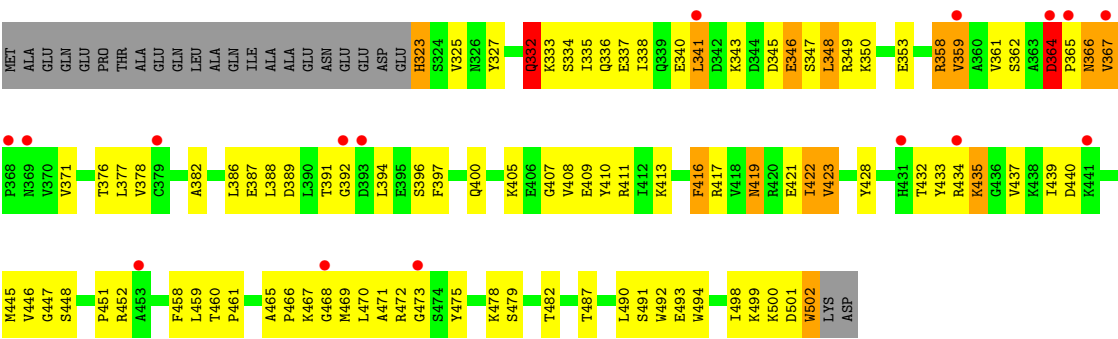


• Molecule 2: RHO GDP-DISSOCIATION INHIBITOR 1





● Molecule 2: RHO GDP-DISSOCIATION INHIBITOR 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.70Å 88.70Å 62.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.70 19.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.1 (19.80-2.70) 84.8 (19.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.68Å)	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 ²)	47.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GER, GDP, 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	0.63	1/1480 (0.1%)	1.07	4/2015 (0.2%)
1	B	0.61	1/1478 (0.1%)	1.15	10/2015 (0.5%)
2	D	0.60	0/1472	1.10	10/1990 (0.5%)
2	E	0.56	1/1472 (0.1%)	1.03	10/1989 (0.5%)
All	All	0.60	3/5902 (0.1%)	1.09	34/8009 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	ASP	C-N	5.79	1.41	1.33
1	A	97	TRP	NE1-CE2	-5.21	1.31	1.37
1	B	97	TRP	NE1-CE2	-5.13	1.31	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	469	MET	N-CA-C	-8.70	102.67	113.20
2	D	315	ALA	N-CA-C	-8.30	101.59	113.21
2	E	469	MET	N-CA-C	-7.67	104.06	113.19
1	B	182	VAL	N-CA-C	7.49	118.38	107.75
1	B	97	TRP	N-CA-C	7.39	119.03	110.97
1	B	179	PRO	O-C-N	-7.33	117.70	121.15
1	A	97	TRP	N-CA-C	7.01	118.71	111.14
1	B	170	ASP	N-CA-C	-6.86	103.03	111.40
2	E	323	HIS	CA-CB-CG	-6.68	107.12	113.80
1	B	187	ARG	N-CA-C	-6.52	102.49	112.99
2	D	329	PRO	CA-C-N	6.50	126.27	119.76
2	D	329	PRO	C-N-CA	6.50	126.27	119.76
2	D	463	GLU	N-CA-C	6.17	117.26	108.74
2	E	359	VAL	O-C-N	6.14	130.25	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	385	PRO	CA-C-N	6.04	130.26	121.26
2	D	385	PRO	C-N-CA	6.04	130.26	121.26
1	B	177	LEU	CB-CA-C	-5.90	102.39	111.83
2	D	447	GLY	N-CA-C	5.83	119.17	111.70
1	A	170	ASP	N-CA-C	-5.81	104.54	111.69
2	D	316	ALA	N-CA-CB	5.76	120.22	110.49
2	E	419	ASN	N-CA-C	5.70	119.94	112.13
1	A	35	THR	N-CA-C	-5.69	104.98	111.07
2	E	447	GLY	N-CA-C	5.46	118.69	111.70
2	D	317	GLU	N-CA-C	-5.44	103.98	111.81
1	B	177	LEU	N-CA-C	5.41	117.93	108.52
2	E	332	GLN	N-CA-C	5.40	116.93	109.15
2	E	358	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	E	467	LYS	N-CA-C	-5.30	102.20	110.42
1	B	106	PRO	N-CA-C	-5.14	103.70	111.41
2	E	359	VAL	CA-C-N	5.08	131.25	121.54
2	E	359	VAL	C-N-CA	5.08	131.25	121.54
1	B	178	CYS	N-CA-C	5.06	121.00	109.81
1	B	63	ASP	N-CA-C	-5.06	105.47	111.69
1	A	96	LYS	N-CA-C	5.01	118.84	112.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1448	0	1473	73	0
1	B	1446	0	1455	128	0
2	D	1445	0	1385	69	0
2	E	1441	0	1426	99	0
3	A	28	0	12	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	356	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 (356) 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:HD2	1:B:183:LYS:N	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
2:E:434:ARG:HE	2:E:435:LYS:HE3	1.46	0.80
2:D:434:ARG:HH11	2:D:434:ARG:HG2	1.46	0.80
1:B:183:LYS:HD2	1:B:183:LYS:H	1.42	0.80
1:B:53:LEU:HD13	1:B:173:ILE:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:353:GLU:CD	2:E:358:ARG:NH1	2.42	0.77
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:E:353:GLU:CD	2:E:358:ARG:HH12	1.93	0.75
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:102:ARG:HB2	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:CD	2:E:422:ILE:H	2.07	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:364:ASP:OD1	2:E:364:ASP:C	2.44	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:HA	1:B:102:ARG:HH11	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
2:D:421:GLU:CD	2:D:422:ILE:H	2.11	0.58
1:B:80:ILE:CD1	1:B:101:VAL:HG21	2.32	0.58
2:D:342:ASP:HB2	2:D:348:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:B:124:ASP:N	2.30	0.57
2:D:468:GLY:C	2:D:470:LEU:H	2.11	0.57
2:E:376:THR:HB	2:E:413:LYS:HB3	1.85	0.57
2:E:468:GLY:C	2:E:470:LEU:H	2.09	0.57
1:B:118:ASP:OD2	1:B:158:SER:HB2	2.05	0.56
2:D:390:LEU:HD22	2:D:490:LEU:HD21	1.86	0.56
2:D:411:ARG:NH1	2:D:462:VAL:HG22	2.21	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:B:11:ASP:CG	1:B:92:ASN:HD22	2.14	0.56
2:E:346:GLU:CD	2:E:350:LYS:HE3	2.30	0.56
2:E:366:ASN:CG	2:E:367:VAL:N	2.59	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
1:A:20:LEU:CD1	1:A:57:ASP:HB2	2.35	0.55
1:A:125:THR:O	1:A:129:LEU:HB2	2.06	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:40:TYR:HD2	1:B:55:LEU:HD12	1.72	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
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
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
2:E:366:ASN:O	2:E:367:VAL:C	2.51	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:E:389:ASP:OD1	2:E:391:THR:OG1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:386:LEU:HD12	2:E:386:LEU:N	2.22	0.53
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:E:361:VAL:HG11	2:E:419:ASN:O	2.08	0.53
2:E:468:GLY:C	2:E:470:LEU:N	2.67	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:366:ASN:C	2:E:366:ASN:ND2	2.65	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
2:D:434:ARG:O	2:D:435:LYS:HB2	2.08	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:HG22	1:B:79:LEU:HD12	1.92	0.52
1:B:8:VAL:HG21	1:B:20:LEU:HD21	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:A:98:TYR:N	1:A:99:PRO:HD2	2.25	0.51
2:D:389:ASP:C	2:D:391:THR:H	2.19	0.51
1:B:103:HIS:O	2:E:445:MET:HE3	2.11	0.51
2:E:411:ARG:HD3	2:E:459:LEU:HB3	1.93	0.51
2:E:416:PHE:CD1	2:E:416:PHE:N	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:O	1:B:163:ARG:HG2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD23	1:B:111:ILE:HB	1.94	0.50
1:B:96:LYS:C	1:B:99:PRO:HD2	2.36	0.50
1:B:9:VAL:HG11	1:B:72:TYR:OH	2.12	0.50
1:B:68:ARG:HB3	1:B:68:ARG:NH1	2.27	0.49
1:B:122:ASP:O	1:B:126:ILE:HG13	2.12	0.49
1:B:76:ASP:O	1:B:109:PRO:HD2	2.12	0.49
1:B:66:ARG:NH1	2:E:332:GLN:OE1	2.45	0.49
1:A:67:LEU:C	1:A:67:LEU:HD23	2.37	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:A:47:ASP:CG	1:A:174:ARG:HH11	2.21	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:7:VAL:HG22	1:A:75:THR:HG21	1.93	0.48
1:A:67:LEU:HD23	1:A:68:ARG:N	2.29	0.48
1:A:87:PRO:CG	1:A:134:LEU:HD12	2.43	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
2:E:434:ARG:C	2:E:435:LYS:HG3	2.39	0.48
1:B:175:ALA:O	1:B:179:PRO:CG	2.62	0.48
2:D:468:GLY:C	2:D:470:LEU:N	2.68	0.48
2:E:335:ILE:O	2:E:338:ILE:HB	2.14	0.47
1:B:181:PRO:C	1:B:182:VAL:CG2	2.86	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:337:GLU:HA	2:E:340:GLU:HG2	1.97	0.47
2:E:411:ARG:HG2	2:E:459:LEU:HD22	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:HA	1:A:123:LYS:CE	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
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
1:B:181:PRO:C	1:B:182:VAL:HG23	2.40	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:488:ASP:OD1	2:D:488:ASP:C	2.59	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: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:HG3	2:E:349:ARG:HH11	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
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:O	2:D:323:HIS:ND1	2.49	0.45
2:D:376:THR:HB	2:D:413:LYS:HD3	1.99	0.45
2:E:333:LYS:HE3	2:E:333:LYS:HB2	1.74	0.45
2:D:370:VAL:HG12	2:D:371:VAL:N	2.31	0.45
1:A:67:LEU:HD12	2:D:338:ILE:HG21	2.00	0.44
1:B:65:ASP:CG	1:B:96:LYS:HZ1	2.25	0.44
1:B:97:TRP:O	1:B:101:VAL:HG23	2.17	0.44
1:B:126:ILE:O	1:B:126:ILE:HG22	2.17	0.44
1:B:61:GLN:CD	1:B:61:GLN:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:18:CYS:SG	1:A:33:ILE:HD13	2.57	0.44
1:B:61:GLN:C	1:B:63:ASP:H	2.24	0.44
1:B:111:ILE:CD1	1:B:172:ALA:HA	2.46	0.44
1:B:166:LYS:HG3	1:B:167:THR:N	2.32	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:377:LEU:HD11	2:E:410:TYR:CD2	2.54	0.43
2:E:387:GLU:CG	2:E:388:LEU:N	2.80	0.43
1:B:116:LYS:HB3	1:B:119:LEU:HD12	2.01	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
2:E:366:ASN:CG	2:E:367:VAL:H	2.24	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:61:GLN:CD	1:B:61:GLN:H	2.27	0.43
1:B:80:ILE:HD11	1:B:101:VAL:HG21	2.00	0.43
2:D:319:GLU:O	2:D:320:GLU:C	2.62	0.43
1:B:131:GLU:O	1:B:131:GLU:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:CD	1:A:61:GLN:H	2.27	0.42
2:D:390:LEU:HD13	2:D:490:LEU:HD23	2.00	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
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
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:E:366:ASN:C	2:E:366:ASN:HD22	2.27	0.42
1:A:187:ARG:O	1:A:188:LYS:C	2.62	0.41
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:177:LEU:C	1:B:178:CYS:SG	2.92	0.41
1:B:138:THR:OG1	1:B:140:PRO:HG2	2.20	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
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:24:THR:CG2	1:B:40:TYR:CE2	3.03	0.41
1:B:182:VAL:HG12	1:B:183:LYS:H	1.81	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:CD1	2:D:416:PHE:N	2.88	0.41
1:A:126:ILE:HG22	1:A:130:LYS:HD2	2.03	0.41
2:E:446:VAL:HG13	2:E:458:PHE:CD2	2.56	0.41
1:B:139:TYR:CD1	1:B:139:TYR:C	2.99	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:5:LYS:HE3	1:A:56:TRP:NE1	2.35	0.40
1:A:177:LEU:O	1:A:178:CYS:CB	2.69	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:A:106:PRO:O	1:A:107:ASN:C	2.64	0.40
1:B:74:GLN:NE2	1:B:74:GLN:CA	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/192 (97%)	173 (92%)	11 (6%)	3 (2%)	7	20
1	B	187/192 (97%)	164 (88%)	18 (10%)	5 (3%)	4	10
2	D	182/204 (89%)	148 (81%)	27 (15%)	7 (4%)	2	5
2	E	178/204 (87%)	147 (83%)	23 (13%)	8 (4%)	2	4
All	All	734/792 (93%)	632 (86%)	79 (11%)	23 (3%)	3	8

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

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Mol	Chain	Res	Type
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%)	145 (91%)	15 (9%)	8	21
1	B	159/168 (95%)	143 (90%)	16 (10%)	7	18
2	D	152/180 (84%)	141 (93%)	11 (7%)	13	32
2	E	159/180 (88%)	147 (92%)	12 (8%)	12	31
All	All	630/696 (90%)	576 (91%)	54 (9%)	10	25

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	31	GLU
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	108	THR
1	A	120	ARG
1	A	123	LYS
1	A	129	LEU
1	A	134	LEU
1	A	158	SER
1	A	189	CYS
1	B	31	GLU
1	B	38	ASP
1	B	39	ASN

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Mol	Chain	Res	Type
1	B	63	ASP
1	B	70	LEU
1	B	74	GLN
1	B	102	ARG
1	B	107	ASN
1	B	124	ASP
1	B	134	LEU
1	B	155	LEU
1	B	163	ARG
1	B	166	LYS
1	B	183	LYS
1	B	186	LYS
1	B	189	CYS
2	D	320	GLU
2	D	336	GLN
2	D	338	ILE
2	D	341	LEU
2	D	348	LEU
2	D	358	ARG
2	D	386	LEU
2	D	389	ASP
2	D	413	LYS
2	D	493	GLU
2	D	501	ASP
2	E	323	HIS
2	E	332	GLN
2	E	336	GLN
2	E	346	GLU
2	E	348	LEU
2	E	364	ASP
2	E	409	GLU
2	E	416	PHE
2	E	422	ILE
2	E	423	VAL
2	E	493	GLU
2	E	502	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	39	ASN

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Mol	Chain	Res	Type
1	A	162	GLN
1	B	39	ASN
1	B	74	GLN
1	B	107	ASN
1	B	141	GLN
1	B	162	GLN
2	D	326	ASN
2	D	366	ASN
2	D	400	GLN
2	D	430	GLN
2	E	339	GLN
2	E	366	ASN
2	E	369	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 oligosaccharides 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
5	GER	D	1502	-	19,19,19	1.51	4 (21%)	21,22,22	2.93	11 (52%)
3	GDP	B	1190	4	29,30,30	3.12	14 (48%)	45,47,47	3.58	16 (35%)
5	GER	E	1503	-	19,19,19	1.53	4 (21%)	21,22,22	2.89	12 (57%)
3	GDP	A	1190	4	29,30,30	3.02	14 (48%)	45,47,47	3.60	16 (35%)

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
5	GER	D	1502	-	-	7/20/20/20	-
3	GDP	B	1190	4	-	3/16/32/32	0/3/3/3
5	GER	E	1503	-	-	5/20/20/20	-
3	GDP	A	1190	4	-	3/16/32/32	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1190	GDP	PA-O3A	9.66	1.69	1.59
3	A	1190	GDP	PA-O3A	8.80	1.69	1.59
3	B	1190	GDP	C2-N1	5.72	1.51	1.37
3	B	1190	GDP	O6-C6	5.71	1.34	1.23
3	B	1190	GDP	C8-N9	5.69	1.50	1.37
3	A	1190	GDP	O6-C6	5.61	1.34	1.23
3	A	1190	GDP	C8-N9	5.57	1.50	1.37
3	A	1190	GDP	C2-N1	5.23	1.50	1.37
3	A	1190	GDP	PB-O2B	-4.43	1.38	1.54
3	B	1190	GDP	PB-O2B	-4.13	1.39	1.54
3	A	1190	GDP	O4'-C1'	3.38	1.49	1.42
3	B	1190	GDP	O4'-C1'	3.23	1.49	1.42
3	B	1190	GDP	C8-N7	3.16	1.41	1.32
3	A	1190	GDP	C5-C4	3.11	1.47	1.38
3	A	1190	GDP	C5-N7	-3.02	1.33	1.39
3	B	1190	GDP	C5-N7	-3.00	1.33	1.39
3	B	1190	GDP	C2-N3	-2.83	1.26	1.33
5	D	1502	GER	C10-C8	2.81	1.57	1.51
3	A	1190	GDP	C8-N7	2.78	1.40	1.32
5	E	1503	GER	C10-C8	2.76	1.57	1.51
3	B	1190	GDP	C5-C4	2.74	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1190	GDP	C2-N3	-2.65	1.26	1.33
5	E	1503	GER	C12-C13	2.49	1.38	1.33
3	A	1190	GDP	C6-N1	-2.32	1.34	1.38
5	D	1502	GER	C7-C8	2.27	1.38	1.33
3	A	1190	GDP	PB-O3B	2.24	1.63	1.54
3	B	1190	GDP	O4'-C4'	2.22	1.49	1.45
5	E	1503	GER	C7-C8	2.21	1.38	1.33
3	B	1190	GDP	C3'-C4'	2.17	1.58	1.53
3	B	1190	GDP	PB-O3B	2.16	1.62	1.54
5	E	1503	GER	C5-C3	2.11	1.55	1.51
3	A	1190	GDP	O4'-C4'	2.11	1.49	1.45
5	D	1502	GER	C12-C13	2.09	1.37	1.33
5	D	1502	GER	C5-C3	2.06	1.55	1.51
3	B	1190	GDP	O3'-C3'	2.05	1.48	1.43
3	A	1190	GDP	O3'-C3'	2.00	1.47	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1190	GDP	N9-C8-N7	-11.09	92.83	113.40
3	A	1190	GDP	N9-C8-N7	-10.63	93.69	113.40
3	A	1190	GDP	C8-N7-C5	9.94	121.97	104.26
3	B	1190	GDP	C8-N7-C5	9.83	121.76	104.26
3	A	1190	GDP	C6-C5-N7	9.15	146.94	130.29
3	B	1190	GDP	C6-C5-N7	8.83	146.36	130.29
5	E	1503	GER	C9-C8-C10	6.98	127.35	115.23
5	D	1502	GER	C9-C8-C10	6.91	127.23	115.23
3	A	1190	GDP	C6-C5-C4	-6.45	109.12	118.83
3	A	1190	GDP	N2-C2-N3	6.33	132.03	119.67
3	B	1190	GDP	C6-C5-C4	-6.03	109.76	118.83
3	B	1190	GDP	N2-C2-N3	6.01	131.41	119.67
3	B	1190	GDP	C8-N9-C4	5.99	117.25	106.03
5	D	1502	GER	C20-C18-C19	5.97	128.33	114.59
5	E	1503	GER	C20-C18-C19	5.75	127.82	114.59
3	A	1190	GDP	C8-N9-C4	5.64	116.59	106.03
3	A	1190	GDP	C5-C6-N1	4.99	125.95	113.25
3	B	1190	GDP	C2-N3-C4	4.89	120.72	112.30
3	B	1190	GDP	C5-C6-N1	4.48	124.65	113.25
3	A	1190	GDP	C2-N3-C4	4.45	119.96	112.30
3	A	1190	GDP	N2-C2-N1	-4.34	107.61	116.76
3	B	1190	GDP	C4-C5-N7	-4.29	103.88	110.67
3	B	1190	GDP	C2-N1-C6	-4.26	117.39	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1190	GDP	C4-C5-N7	-4.25	103.93	110.67
3	A	1190	GDP	C2-N1-C6	-4.19	117.51	125.11
3	A	1190	GDP	O6-C6-C5	-4.14	115.61	126.53
5	D	1502	GER	C4-C3-C5	4.12	122.37	115.23
5	E	1503	GER	C4-C3-C5	4.11	122.37	115.23
3	B	1190	GDP	O6-C6-C5	-4.06	115.82	126.53
3	B	1190	GDP	N2-C2-N1	-3.73	108.89	116.76
5	D	1502	GER	C6-C5-C3	3.49	124.75	113.19
3	B	1190	GDP	C2'-C3'-C4'	3.47	109.31	102.61
5	D	1502	GER	C14-C13-C15	3.36	121.06	115.23
5	E	1503	GER	C6-C5-C3	3.28	124.06	113.19
5	E	1503	GER	C14-C13-C15	3.25	120.87	115.23
5	E	1503	GER	C16-C15-C13	3.15	123.62	113.19
3	A	1190	GDP	C2'-C3'-C4'	3.04	108.48	102.61
5	D	1502	GER	C20-C18-C17	-3.02	113.60	122.66
5	D	1502	GER	C16-C15-C13	3.01	123.16	113.19
5	E	1503	GER	C20-C18-C17	-2.94	113.85	122.66
5	D	1502	GER	C11-C10-C8	2.88	122.73	113.19
3	A	1190	GDP	C1'-N9-C8	-2.85	118.62	126.73
3	B	1190	GDP	C1'-N9-C8	-2.73	118.98	126.73
5	D	1502	GER	C10-C8-C7	-2.64	115.24	121.17
5	E	1503	GER	C10-C8-C7	-2.57	115.40	121.17
5	E	1503	GER	C11-C10-C8	2.56	121.66	113.19
5	E	1503	GER	C9-C8-C7	-2.48	117.25	123.63
3	A	1190	GDP	O2'-C2'-C3'	2.42	119.56	111.82
3	B	1190	GDP	O2'-C2'-C3'	2.38	119.45	111.82
5	D	1502	GER	C9-C8-C7	-2.37	117.53	123.63
3	B	1190	GDP	C4'-O4'-C1'	2.32	114.60	109.47
5	D	1502	GER	C6-C7-C8	-2.29	122.39	127.62
5	E	1503	GER	C6-C7-C8	-2.22	122.55	127.62
3	A	1190	GDP	C4'-O4'-C1'	2.16	114.25	109.47
5	E	1503	GER	C11-C12-C13	-2.05	122.93	127.62

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

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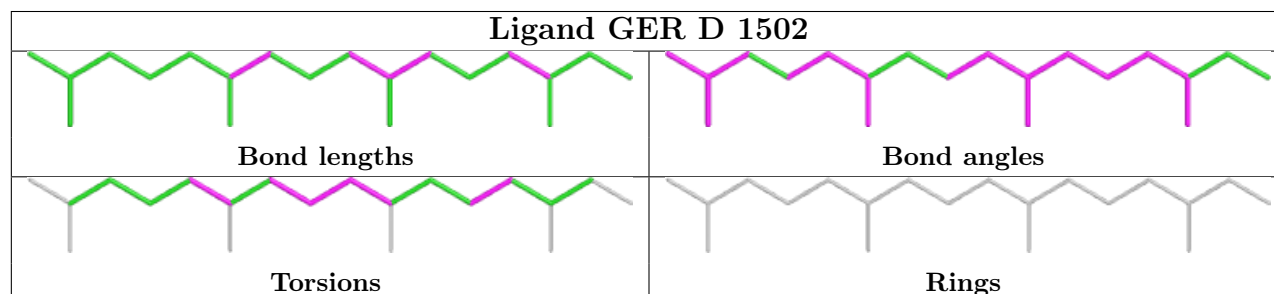
Mol	Chain	Res	Type	Atoms
5	D	1502	GER	C12-C13-C15-C16
5	D	1502	GER	C8-C10-C11-C12
5	E	1503	GER	C4-C3-C5-C6
5	E	1503	GER	C2-C3-C5-C6
5	E	1503	GER	C3-C5-C6-C7
5	D	1502	GER	C3-C5-C6-C7
5	E	1503	GER	C14-C13-C15-C16
3	A	1190	GDP	PA-O3A-PB-O1B
3	B	1190	GDP	PA-O3A-PB-O1B
3	A	1190	GDP	PA-O3A-PB-O3B
3	B	1190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

There are no ring outliers.

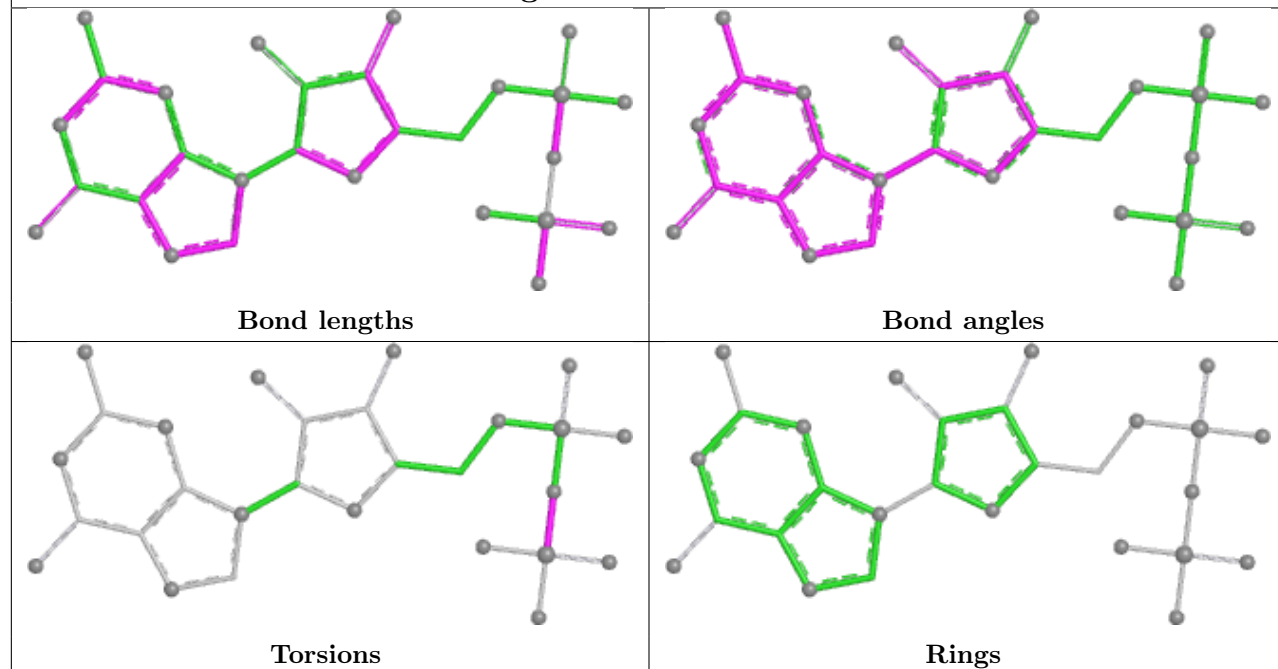
3 monomers are involved in 13 short contacts:

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

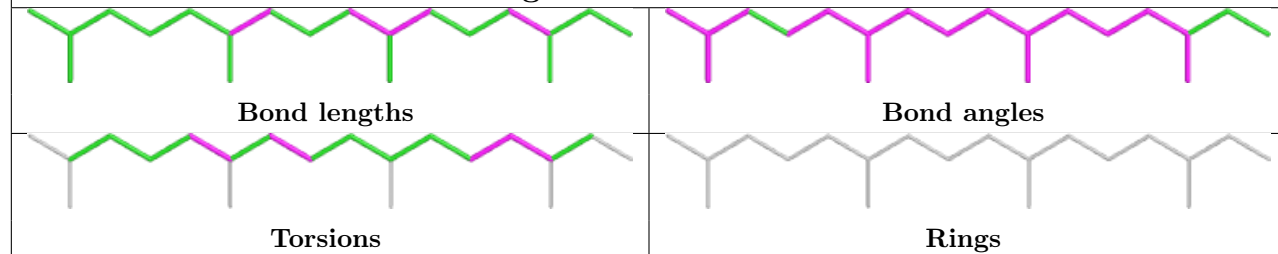
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



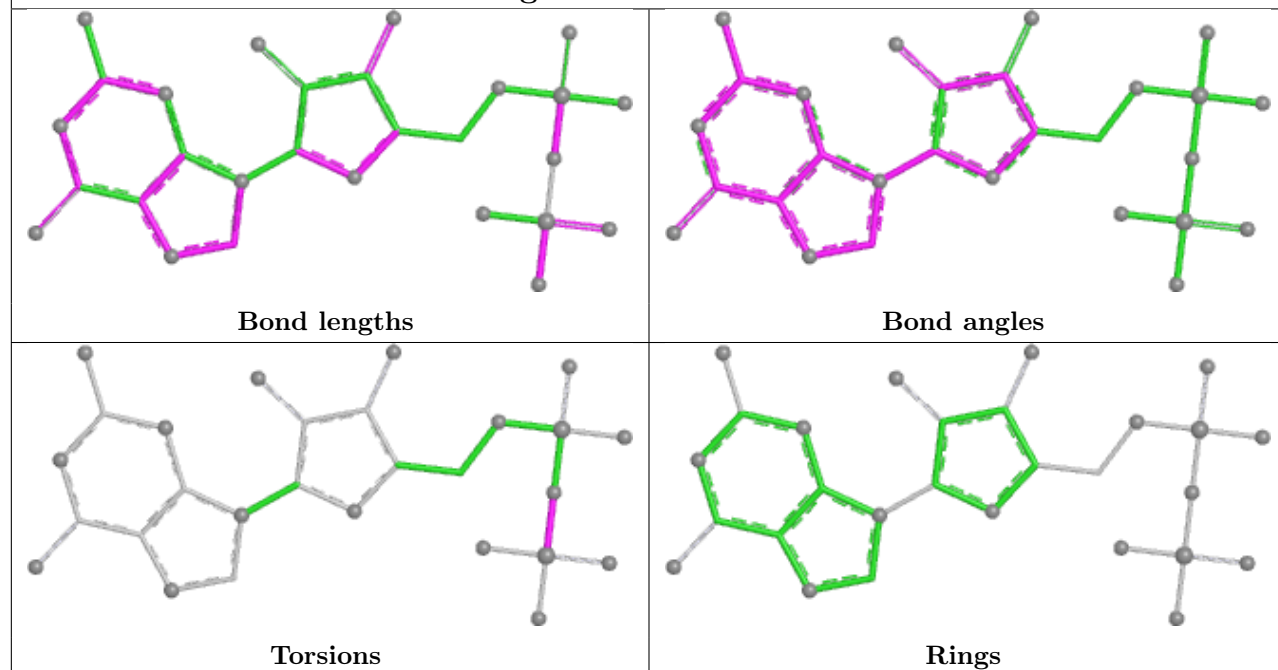
Ligand GDP B 1190



Ligand GER E 1503



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	189/192 (98%)	-0.05	6 (3%)	50	46	4, 31, 98, 132	0
1	B	189/192 (98%)	0.34	11 (5%)	29	25	11, 46, 113, 132	0
2	D	186/204 (91%)	0.81	23 (12%)	8	7	24, 67, 119, 132	0
2	E	180/204 (88%)	0.66	16 (8%)	15	13	21, 68, 110, 132	0
All	All	744/792 (93%)	0.44	56 (7%)	20	17	4, 52, 115, 132	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	475	TYR	4.7
1	A	178	CYS	4.7
1	B	179	PRO	4.2
2	D	341	LEU	4.1
1	B	178	CYS	3.9
2	D	368	PRO	3.9
2	E	359	VAL	3.7
1	B	30	GLY	3.7
1	B	184	LYS	3.6
2	D	407	GLY	3.4
2	D	396	SER	3.3
2	D	497	THR	3.3
2	E	453	ALA	3.3
2	D	439	ILE	3.2
2	E	473	GLY	3.1
2	D	476	SER	3.0
2	E	393	ASP	3.0
2	D	346	GLU	2.9
2	D	473	GLY	2.9
2	E	369	ASN	2.9
1	A	30	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	341	LEU	2.8
1	B	42	ALA	2.7
2	E	367	VAL	2.7
2	D	367	VAL	2.6
1	A	189	CYS	2.6
2	D	382	ALA	2.6
1	B	1	PRO	2.6
1	A	184	LYS	2.5
2	E	441	LYS	2.5
1	A	40	TYR	2.5
1	B	40	TYR	2.5
2	D	358	ARG	2.4
2	D	468	GLY	2.4
1	B	46	VAL	2.4
2	D	498	ILE	2.4
2	D	387	GLU	2.4
1	B	181	PRO	2.4
1	A	182	VAL	2.4
1	B	185	ARG	2.3
2	E	365	PRO	2.3
2	E	392	GLY	2.3
2	D	373	THR	2.2
2	D	322	GLU	2.2
2	D	493	GLU	2.2
2	E	368	PRO	2.2
2	D	397	PHE	2.2
1	B	189	CYS	2.2
2	E	364	ASP	2.2
2	E	434	ARG	2.2
2	D	317	GLU	2.2
2	E	468	GLY	2.2
2	E	431	HIS	2.2
2	E	379	CYS	2.1
2	D	314	ILE	2.1
2	D	316	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

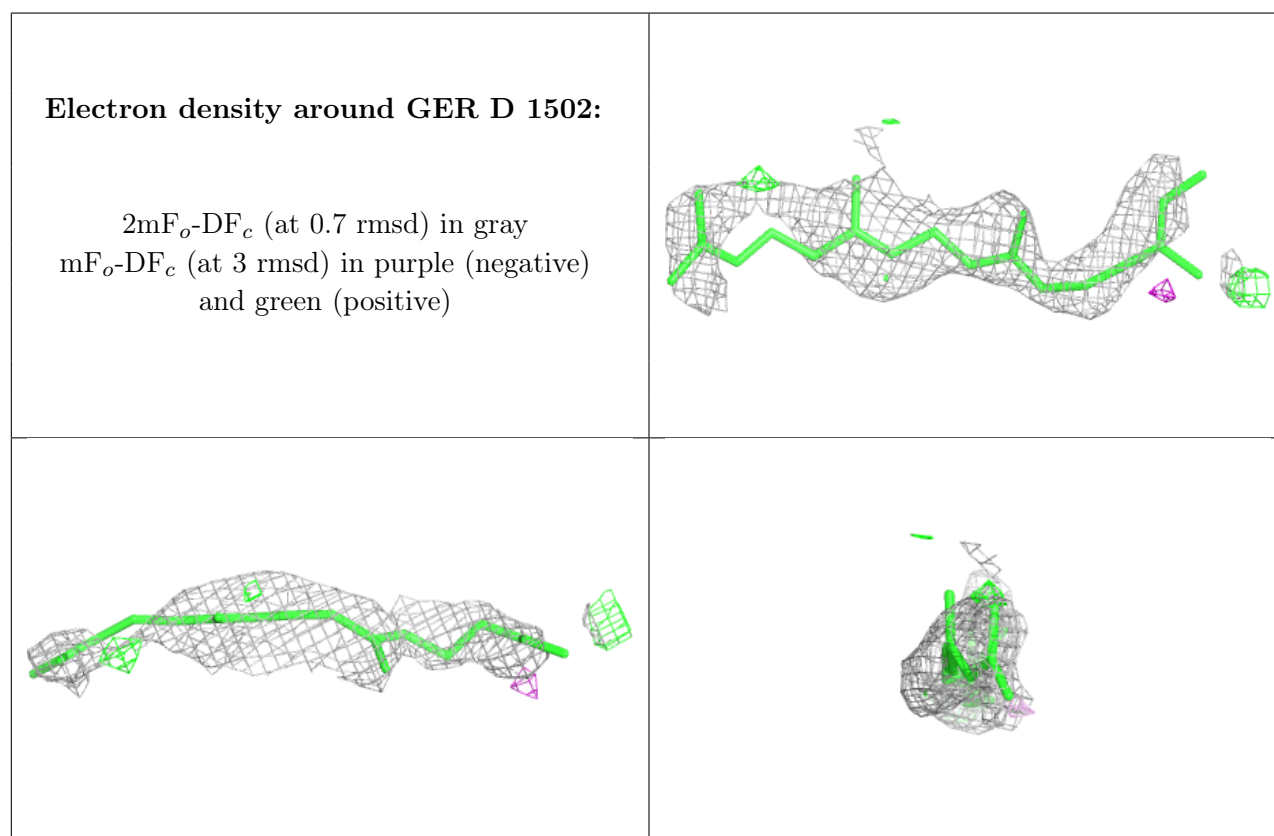
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

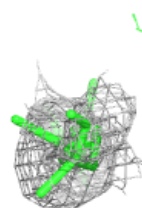
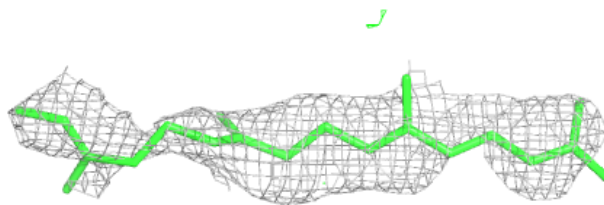
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GER	D	1502	20/20	0.76	0.19	78,78,78,78	0
5	GER	E	1503	20/20	0.77	0.16	78,78,78,78	0
4	MG	B	1191	1/1	0.87	0.39	48,48,48,48	0
3	GDP	B	1190	28/28	0.92	0.09	48,48,48,48	0
4	MG	A	1191	1/1	0.93	0.15	48,48,48,48	0
3	GDP	A	1190	28/28	0.97	0.09	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.

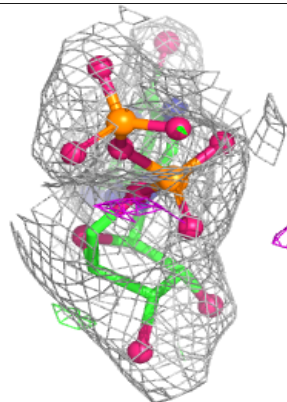
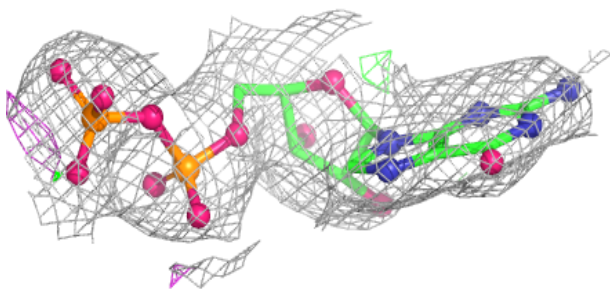
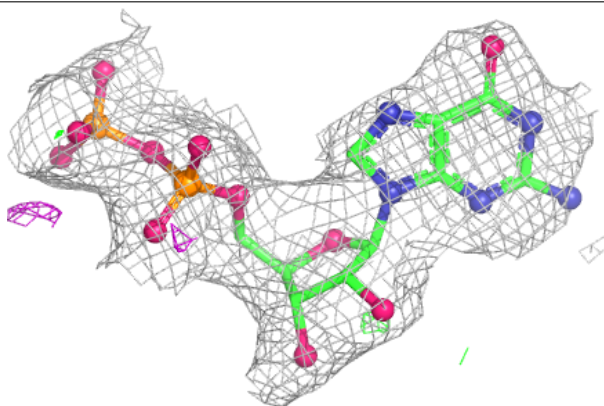


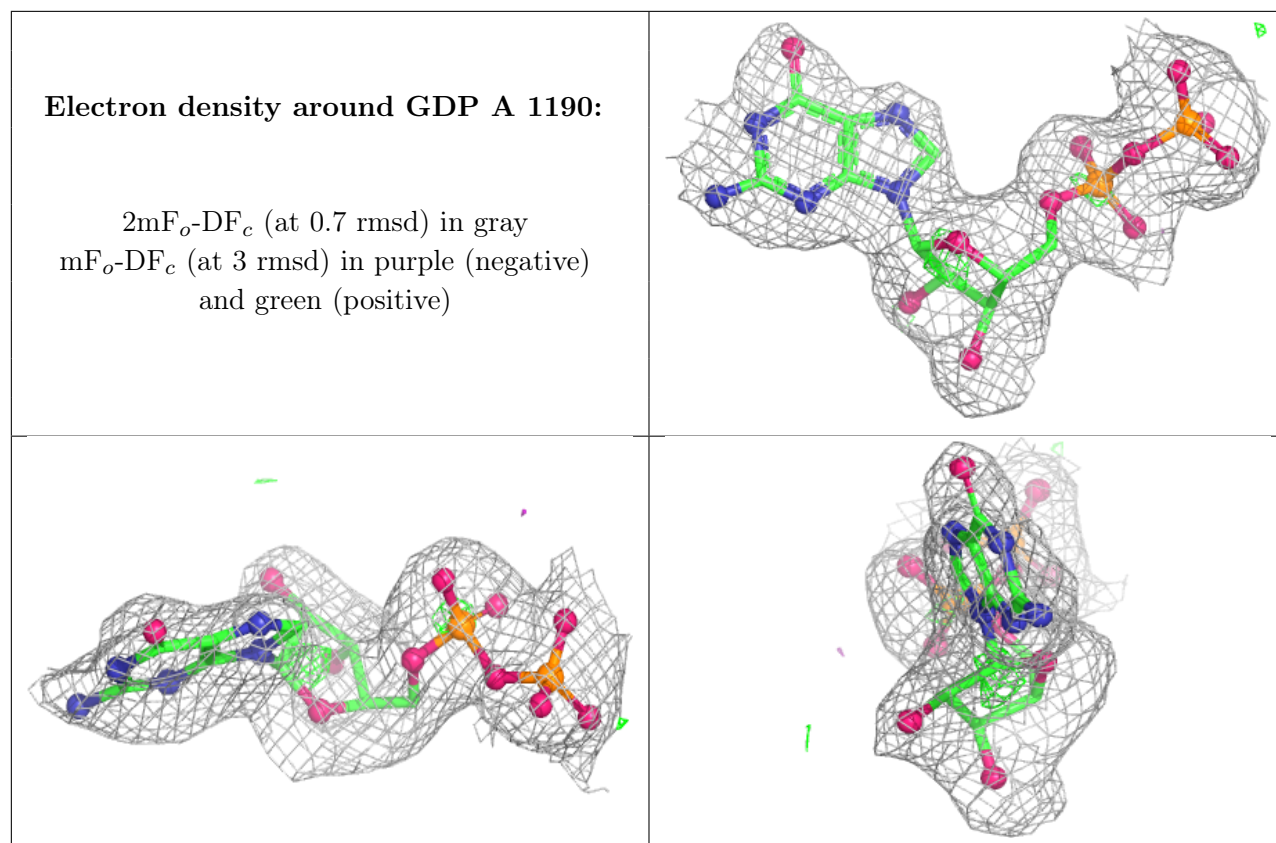
Electron density around GER E 1503:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.