



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:37 PM UTC

PDB ID : 1HOP / pdb_00001hop
Title : STRUCTURE OF GUANINE NUCLEOTIDE (GPPCP) COMPLEX OF ADENYLOSUCCINATE SYNTHETASE FROM ESCHERICHIA COLI AT PH 6.5 AND 25 DEGREES CELSIUS
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Deposited on : 1996-04-26
Resolution : 2.30 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

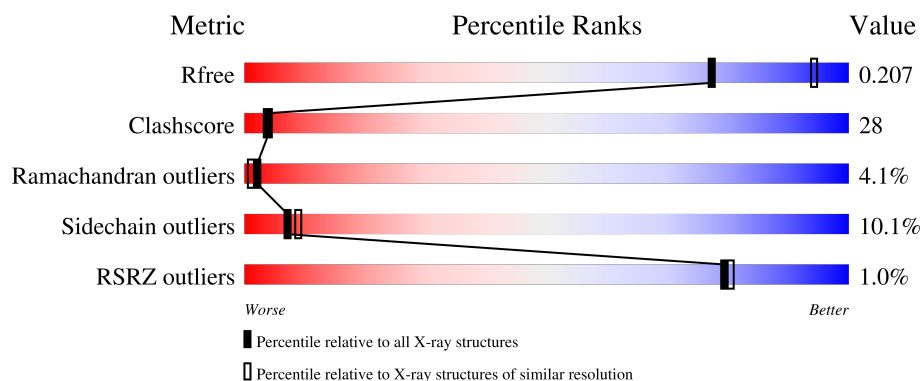
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	431	2% 45% 45% 9%
1	B	431	49% 41% 8%

2 Entry composition [i](#)

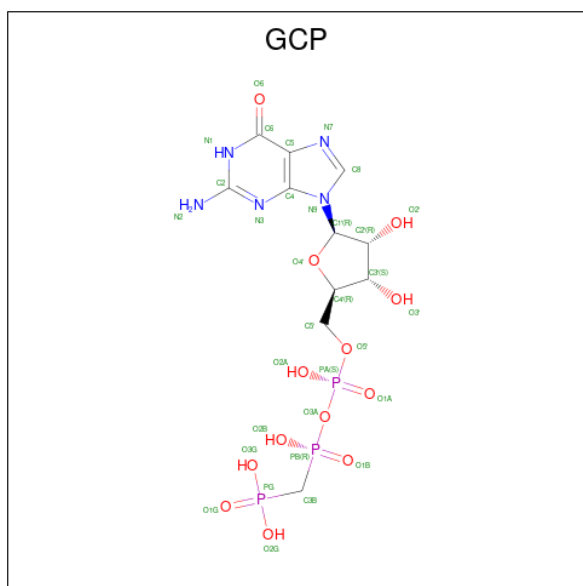
There are 3 unique types of molecules in this entry. The entry contains 9261 atoms, of which 2210 are hydrogens and 0 are deuteriums.

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 ADENYLOSUCCINATE SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total	C	H	N	O	S	0	0	0
			4069	2092	748	576	640	13			
1	B	431	Total	C	H	N	O	S	0	0	0
			4069	2092	748	576	640	13			

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			44	11	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			44	11	12	5	13	3		

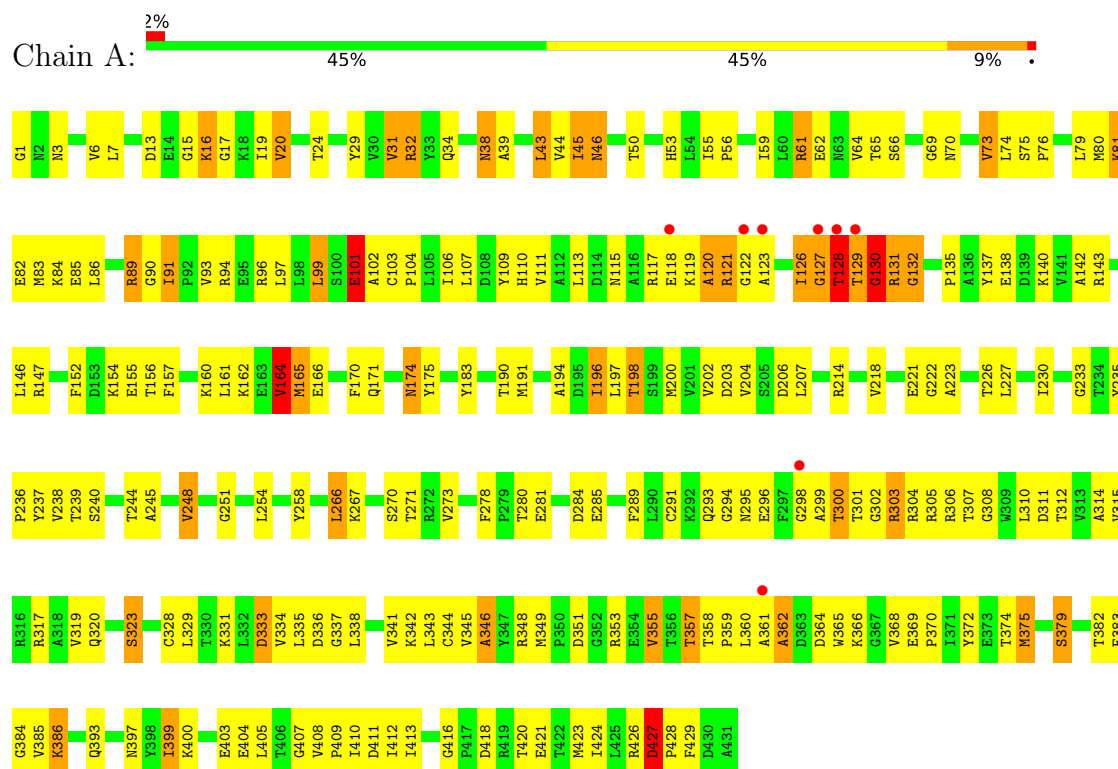
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	162	Total 486	H 324	O 162	0	0
3	B	183	Total 549	H 366	O 183	0	0

3 Residue-property plots

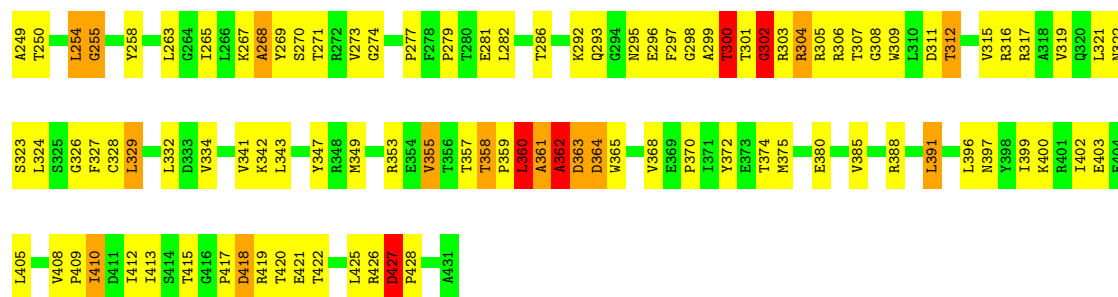
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ADENYLOSUCCINATE SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.85Å 94.06Å 119.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 15.00 – 2.32	Depositor EDS
% Data completeness (in resolution range)	70.0 (15.00-2.30) 64.0 (15.00-2.32)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.32Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , 0.227 0.192 , 0.207	Depositor DCC
R_{free} test set	2343 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9261	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 27.40 % 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 2.2155e-03.*

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: GCP

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	1.08	5/3379 (0.1%)	1.33	37/4577 (0.8%)
1	B	1.09	6/3379 (0.2%)	1.33	33/4577 (0.7%)
All	All	1.08	11/6758 (0.2%)	1.33	70/9154 (0.8%)

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	A	0	3
1	B	0	2
All	All	0	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ILE	C-N	25.55	1.70	1.33
1	B	300	THR	C-N	24.47	1.68	1.33
1	A	130	GLY	C-N	20.58	1.62	1.33
1	B	360	LEU	C-N	6.31	1.42	1.33
1	B	410	ILE	CA-CB	6.17	1.62	1.54
1	A	73	VAL	CA-C	5.96	1.59	1.52
1	B	362	ALA	C-N	5.70	1.41	1.33
1	B	402	ILE	CA-CB	5.51	1.60	1.54
1	A	106	ILE	CA-CB	5.26	1.60	1.54
1	B	68	ILE	CA-CB	5.14	1.59	1.53
1	A	413	ILE	CA-CB	5.01	1.60	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	GLY	O-C-N	-15.55	103.14	122.58
1	B	302	GLY	CA-C-N	-12.23	103.63	121.24
1	B	302	GLY	C-N-CA	-12.23	103.63	121.24
1	A	285	GLU	N-CA-C	10.90	122.91	111.14
1	A	126	ILE	O-C-N	-10.57	109.36	122.57
1	B	255	GLY	CA-C-N	10.52	130.72	119.05
1	B	255	GLY	C-N-CA	10.52	130.72	119.05
1	B	427	ASP	CA-C-N	9.14	128.75	119.24
1	B	427	ASP	C-N-CA	9.14	128.75	119.24
1	A	204	VAL	N-CA-C	8.36	118.41	110.30
1	A	369	GLU	CA-C-N	8.21	128.69	119.83
1	A	369	GLU	C-N-CA	8.21	128.69	119.83
1	B	364	ASP	N-CA-C	7.95	127.72	110.80
1	A	129	THR	CB-CA-C	-7.73	101.92	111.82
1	B	7	LEU	N-CA-C	7.60	120.41	108.79
1	A	251	GLY	N-CA-C	7.35	122.87	113.24
1	A	399	ILE	CB-CA-C	-6.84	103.21	111.97
1	A	375	MET	CA-C-N	6.72	126.76	119.90
1	A	375	MET	C-N-CA	6.72	126.76	119.90
1	B	148	VAL	CB-CA-C	-6.70	102.97	112.22
1	B	74	LEU	N-CA-C	6.57	119.95	109.24
1	B	250	THR	N-CA-C	6.54	118.07	111.07
1	A	233	GLY	N-CA-C	6.54	122.64	111.98
1	A	69	GLY	N-CA-C	6.46	123.56	112.51
1	B	317	ARG	N-CA-C	-6.45	103.94	110.97
1	B	363	ASP	N-CA-C	-6.37	100.73	109.71
1	A	17	GLY	N-CA-C	6.30	120.52	112.83
1	B	402	ILE	N-CA-C	-6.21	104.46	110.42
1	B	134	GLY	CA-C-N	6.05	127.40	119.84
1	B	134	GLY	C-N-CA	6.05	127.40	119.84
1	A	31	VAL	N-CA-C	6.02	116.78	108.12
1	A	278	PHE	CA-C-N	5.90	126.32	119.47
1	A	278	PHE	C-N-CA	5.90	126.32	119.47
1	A	319	VAL	CB-CA-C	-5.90	104.31	112.04
1	B	113	LEU	N-CA-C	-5.90	103.55	112.04
1	A	103	CYS	CA-C-N	5.87	125.62	119.76
1	A	103	CYS	C-N-CA	5.87	125.62	119.76
1	A	266	LEU	N-CA-C	5.76	117.76	107.80
1	B	157	PHE	N-CA-C	-5.68	105.00	111.14
1	A	355	VAL	N-CA-C	5.65	116.02	108.11
1	A	248	VAL	N-CA-C	5.61	116.39	110.72
1	B	67	ILE	CA-C-N	-5.53	115.56	122.48
1	B	67	ILE	C-N-CA	-5.53	115.56	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	TYR	N-CA-C	5.53	118.27	110.14
1	A	323	SER	N-CA-C	-5.50	103.64	111.24
1	A	174	ASN	N-CA-C	5.47	117.05	111.14
1	B	173	VAL	N-CA-C	5.37	117.27	111.58
1	A	32	ARG	N-CA-C	-5.34	100.59	109.46
1	B	16	LYS	N-CA-C	5.34	117.10	111.28
1	B	228	LEU	N-CA-C	-5.33	105.42	112.94
1	B	226	THR	N-CA-C	5.30	120.12	111.37
1	B	297	PHE	N-CA-C	-5.29	101.66	110.17
1	A	101	GLU	N-CA-C	-5.23	105.64	112.23
1	A	91	ILE	CB-CA-C	-5.23	104.88	110.16
1	A	164	VAL	CB-CA-C	-5.22	105.29	111.97
1	A	427	ASP	CA-C-N	5.22	125.27	119.32
1	A	427	ASP	C-N-CA	5.22	125.27	119.32
1	B	38	ASN	CB-CA-C	-5.22	101.65	110.88
1	A	221	GLU	N-CA-C	5.20	116.99	108.52
1	B	358	THR	CA-C-N	-5.19	114.45	119.90
1	B	358	THR	C-N-CA	-5.19	114.45	119.90
1	A	222	GLY	N-CA-C	-5.14	103.34	112.54
1	A	128	THR	CA-C-N	-5.11	114.84	122.36
1	A	128	THR	C-N-CA	-5.11	114.84	122.36
1	B	297	PHE	O-C-N	-5.11	117.23	123.10
1	A	429	PHE	N-CA-C	5.09	118.59	112.38
1	B	106	ILE	N-CA-C	-5.07	101.11	108.36
1	A	370	PRO	N-CA-C	5.06	118.83	111.03
1	B	363	ASP	CA-C-N	5.02	131.13	121.54
1	B	363	ASP	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	GLY	Peptide,Mainchain
1	A	237	TYR	Sidechain
1	B	302	GLY	Mainchain
1	B	362	ALA	Mainchain

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	3321	748	3325	192	0
1	B	3321	748	3326	187	0
2	A	32	12	14	1	0
2	B	32	12	14	3	0
3	A	162	324	0	13	0
3	B	183	366	0	18	0
All	All	7051	2210	6679	374	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 28.

All (374) 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:300:THR:C	1:B:301:THR:N	1.68	1.48
1:A:126:ILE:C	1:A:127:GLY:N	1.70	1.47
1:A:129:THR:HG22	1:A:129:THR:O	1.64	0.94
1:A:16:LYS:HD2	3:A:543:HOH:O	1.70	0.91
1:A:128:THR:CG2	1:A:128:THR:O	2.20	0.90
1:A:226:THR:HG23	1:A:244:THR:HG22	1.58	0.86
1:A:81:LYS:HE2	1:A:81:LYS:HA	1.61	0.82
1:A:101:GLU:HG3	1:A:102:ALA:N	1.95	0.82
3:A:479:HOH:O	1:B:235:TYR:HE2	1.65	0.79
1:A:46:ASN:HB3	1:A:89:ARG:HG3	1.65	0.79
1:A:128:THR:O	1:A:128:THR:HG22	1.82	0.78
1:A:384:GLY:HA2	1:A:421:GLU:HG3	1.63	0.78
1:B:311:ASP:O	1:B:315:VAL:HG23	1.83	0.78
1:A:271:THR:HG22	1:A:307:THR:HG22	1.67	0.77
1:A:349:MET:SD	1:A:368:VAL:HG12	2.25	0.76
1:A:131:ARG:HH11	1:A:131:ARG:HB3	1.50	0.75
1:B:31:VAL:HG22	1:B:67:ILE:HD12	1.66	0.75
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.51	0.75
1:A:399:ILE:HG23	1:A:410:ILE:HD12	1.68	0.75
1:A:109:TYR:O	1:A:113:LEU:HD23	1.87	0.74
3:A:524:HOH:O	1:B:143:ARG:HD3	1.87	0.73
1:B:235:TYR:O	1:B:238:VAL:HG22	1.87	0.73
1:B:61:ARG:HD2	3:B:593:HOH:O	1.89	0.73
1:B:244:THR:HB	1:B:322:ASN:OD1	1.89	0.72
1:A:56:PRO:HB2	1:A:66:SER:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HG2	1:A:191:MET:HE1	1.72	0.72
1:A:426:ARG:O	1:A:427:ASP:HB3	1.89	0.72
1:B:282:LEU:HG	1:B:308:GLY:HA2	1.71	0.71
1:A:46:ASN:CB	1:A:89:ARG:HG3	2.19	0.71
1:A:128:THR:O	1:A:129:THR:HB	1.89	0.71
1:A:89:ARG:HD3	1:A:89:ARG:N	2.05	0.71
1:B:334:VAL:HA	3:B:439:HOH:O	1.91	0.71
1:B:312:THR:HG21	1:B:405:LEU:HB3	1.73	0.71
1:B:360:LEU:HD23	1:B:360:LEU:H	1.54	0.70
1:B:319:VAL:HA	1:B:324:LEU:HD12	1.73	0.70
1:A:115:ASN:OD1	1:A:130:GLY:HA2	1.91	0.70
1:A:162:LYS:O	1:A:166:GLU:HG3	1.92	0.69
1:B:328:CYS:SG	1:B:412:ILE:HG22	2.31	0.69
1:A:117:ARG:HH12	1:A:135:PRO:HG3	1.57	0.69
1:A:39:ALA:HA	1:A:223:ALA:HB1	1.73	0.69
1:A:129:THR:O	1:A:129:THR:CG2	2.37	0.69
1:B:9:THR:HG21	1:B:327:PHE:HE1	1.57	0.69
1:A:305:ARG:HD3	3:A:471:HOH:O	1.92	0.68
1:B:99:LEU:HD11	1:B:200:MET:HE3	1.75	0.68
1:A:97:LEU:HB3	1:A:200:MET:HE3	1.75	0.68
1:A:310:LEU:HD23	1:A:343:LEU:CD2	2.24	0.67
1:A:335:LEU:HD13	1:A:341:VAL:HG11	1.76	0.67
1:A:203:ASP:OD2	1:A:206:ASP:HB2	1.95	0.67
1:A:131:ARG:HB3	1:A:131:ARG:NH1	2.09	0.67
1:B:129:THR:HA	1:B:131:ARG:NH1	2.09	0.67
1:B:300:THR:C	1:B:301:THR:CA	2.64	0.67
1:B:397:ASN:HA	1:B:400:LYS:NZ	2.09	0.67
1:B:20:VAL:O	1:B:24:THR:HG23	1.95	0.66
1:A:19:ILE:HD12	1:A:19:ILE:H	1.60	0.66
1:A:254:LEU:HD12	3:A:472:HOH:O	1.94	0.66
1:B:85:GLU:O	1:B:89:ARG:HG2	1.96	0.66
1:B:32:ARG:HG3	1:B:32:ARG:NH1	2.11	0.65
1:B:302:GLY:O	1:B:303:ARG:C	2.40	0.65
1:B:281:GLU:HA	1:B:307:THR:O	1.97	0.65
1:A:345:VAL:HG12	1:A:405:LEU:HD13	1.78	0.65
1:B:142:ALA:O	1:B:143:ARG:C	2.40	0.64
1:B:349:MET:HE1	1:B:368:VAL:HG22	1.79	0.64
1:A:245:ALA:O	1:A:248:VAL:HG23	1.97	0.64
1:A:117:ARG:NH1	1:A:135:PRO:HG3	2.12	0.64
1:A:152:PHE:CZ	1:A:198:THR:HG22	2.32	0.64
1:B:99:LEU:CD1	1:B:200:MET:HE3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:O	1:A:119:LYS:C	2.40	0.64
1:B:41:HIS:CE1	1:B:57:SER:HB3	2.33	0.64
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.62	0.63
1:B:397:ASN:CG	1:B:400:LYS:HZ1	2.04	0.63
1:A:62:GLU:HA	1:A:96:ARG:NH1	2.13	0.63
1:A:55:ILE:HG12	1:A:82:GLU:OE1	1.97	0.63
1:B:18:LYS:HE3	1:B:419:ARG:HA	1.81	0.63
1:A:97:LEU:HD23	1:A:200:MET:CE	2.28	0.62
1:B:234:THR:HG21	1:B:277:PRO:HD2	1.80	0.62
1:A:293:GLN:HB3	1:A:334:VAL:HG13	1.82	0.62
1:B:388:ARG:HH11	1:B:425:LEU:HD22	1.66	0.61
1:A:19:ILE:HD12	1:A:19:ILE:N	2.15	0.61
1:A:101:GLU:CD	1:A:147:ARG:HH21	2.08	0.61
1:A:19:ILE:HG12	1:A:328:CYS:SG	2.41	0.60
1:A:43:LEU:HD12	1:A:50:THR:O	2.01	0.60
1:B:249:ALA:HA	1:B:254:LEU:O	2.00	0.60
1:A:73:VAL:HG12	1:A:104:PRO:HB2	1.83	0.60
1:B:286:THR:HG21	1:B:309:TRP:CH2	2.36	0.60
1:A:258:TYR:CE2	1:B:323:SER:HB3	2.37	0.60
1:B:299:ALA:O	1:B:300:THR:HB	2.00	0.60
1:B:349:MET:HG3	1:B:353:ARG:NH2	2.16	0.60
1:A:128:THR:O	1:A:128:THR:HG23	1.99	0.59
1:B:328:CYS:SG	1:B:412:ILE:CG2	2.91	0.59
1:B:128:THR:O	1:B:128:THR:HG23	2.03	0.59
1:A:128:THR:HG21	3:A:438:HOH:O	2.02	0.59
1:A:345:VAL:O	1:A:346:ALA:HB2	2.01	0.59
1:B:277:PRO:HB3	1:B:365:TRP:HB3	1.84	0.59
1:A:90:GLY:C	1:A:91:ILE:HD12	2.27	0.58
1:A:160:LYS:O	1:A:164:VAL:HG23	2.03	0.58
1:B:45:ILE:HD13	1:B:60:LEU:HD11	1.85	0.58
1:B:42:THR:HG23	3:B:539:HOH:O	2.04	0.58
1:B:184:GLN:HE22	1:B:187:LEU:HD23	1.69	0.58
1:B:83:MET:O	1:B:87:GLU:HG3	2.02	0.58
1:B:186:VAL:HG13	3:B:477:HOH:O	2.04	0.58
1:B:399:ILE:O	1:B:403:GLU:HG3	2.04	0.58
1:A:79:LEU:CD1	1:A:83:MET:SD	2.92	0.58
1:A:365:TRP:O	1:A:368:VAL:HG22	2.03	0.58
1:A:301:THR:HB	1:A:303:ARG:NH2	2.19	0.57
1:A:74:LEU:CD2	1:A:99:LEU:HD22	2.34	0.57
1:B:235:TYR:O	1:B:236:PRO:C	2.46	0.57
1:B:360:LEU:H	1:B:360:LEU:CD2	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ASN:O	1:B:400:LYS:HG3	2.05	0.57
1:B:129:THR:HA	1:B:131:ARG:CZ	2.35	0.56
1:B:282:LEU:HD11	1:B:309:TRP:NE1	2.20	0.56
1:B:107:LEU:H	1:B:110:HIS:HD2	1.53	0.56
1:A:382:THR:O	1:A:385:VAL:HG23	2.05	0.56
1:A:416:GLY:HA3	1:A:421:GLU:HG2	1.88	0.55
1:A:118:GLU:HG2	1:A:123:ALA:HA	1.88	0.55
1:A:62:GLU:HG3	1:A:96:ARG:HH12	1.70	0.55
1:B:426:ARG:O	1:B:427:ASP:HB3	2.07	0.55
1:A:311:ASP:HA	1:A:344:CYS:HB3	1.89	0.55
1:A:364:ASP:OD1	1:A:366:LYS:HB3	2.06	0.55
1:B:182:ASP:HA	3:B:511:HOH:O	2.07	0.55
1:A:152:PHE:CE1	1:A:198:THR:HG22	2.42	0.55
1:A:1:GLY:HA2	3:A:461:HOH:O	2.06	0.54
1:B:131:ARG:HD2	1:B:133:ILE:HD12	1.90	0.54
1:B:37:HIS:CD2	1:B:37:HIS:H	2.25	0.54
1:A:130:GLY:O	1:A:131:ARG:C	2.49	0.54
1:A:146:LEU:HD22	1:A:157:PHE:CE1	2.43	0.54
1:B:169:ASN:O	1:B:173:VAL:HG22	2.08	0.54
1:B:9:THR:HG21	1:B:327:PHE:CE1	2.42	0.53
1:B:114:ASP:HB3	1:B:130:GLY:HA2	1.89	0.53
1:A:312:THR:HG21	1:A:405:LEU:HB3	1.89	0.53
1:A:418:ASP:HB3	1:A:421:GLU:OE1	2.08	0.53
1:A:15:GLY:HA2	2:A:432:GCP:C5'	2.39	0.53
1:A:351:ASP:OD1	1:A:353:ARG:HG2	2.09	0.53
1:B:312:THR:HG21	1:B:405:LEU:CB	2.37	0.53
1:A:384:GLY:HA2	1:A:421:GLU:CG	2.35	0.53
1:B:282:LEU:HD11	1:B:309:TRP:CE2	2.44	0.53
1:A:357:THR:HG22	3:B:607:HOH:O	2.09	0.52
1:B:235:TYR:HB3	1:B:236:PRO:HD3	1.90	0.52
1:B:418:ASP:HB3	1:B:421:GLU:OE1	2.09	0.52
1:B:92:PRO:HB2	1:B:95:GLU:HG2	1.91	0.52
1:A:91:ILE:HD12	1:A:91:ILE:N	2.25	0.52
1:B:117:ARG:NH1	1:B:135:PRO:HG3	2.25	0.52
1:B:157:PHE:CZ	1:B:190:THR:HG21	2.44	0.52
1:A:74:LEU:HD21	1:A:99:LEU:HD22	1.91	0.52
1:A:59:ILE:HG21	1:A:86:LEU:HD13	1.92	0.52
1:A:196:ILE:HG22	1:A:197:LEU:N	2.23	0.52
1:B:129:THR:O	1:B:131:ARG:HG2	2.10	0.52
1:B:45:ILE:HD12	1:B:60:LEU:HD21	1.92	0.52
2:B:433:GCP:H5'1	3:B:480:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLY:O	1:A:303:ARG:C	2.53	0.51
1:B:41:HIS:CE1	1:B:57:SER:CB	2.93	0.51
1:B:374:THR:HG21	3:B:491:HOH:O	2.10	0.51
1:B:273:VAL:HG22	1:B:305:ARG:HG2	1.93	0.51
1:B:359:PRO:HG2	1:B:365:TRP:CD1	2.45	0.51
1:A:3:ASN:ND2	1:A:258:TYR:O	2.44	0.51
1:B:70:ASN:HB2	1:B:102:ALA:HB3	1.92	0.51
1:A:333:ASP:CB	1:A:383:PHE:HD1	2.24	0.51
1:A:29:TYR:HB2	1:A:218:VAL:HG22	1.93	0.51
1:A:75:SER:O	1:A:76:PRO:C	2.50	0.51
1:B:21:ASP:HB3	1:B:419:ARG:HH22	1.76	0.51
1:B:355:VAL:HG22	1:B:357:THR:H	1.75	0.51
1:B:286:THR:HG21	1:B:309:TRP:CZ2	2.45	0.51
1:B:184:GLN:NE2	1:B:187:LEU:HD23	2.25	0.51
1:B:44:VAL:HA	1:B:49:LYS:HA	1.91	0.51
1:B:214:ARG:NH1	1:B:216:ASP:OD2	2.44	0.51
1:A:120:ALA:O	1:A:122:GLY:N	2.44	0.51
1:B:111:VAL:HG22	1:B:131:ARG:O	2.11	0.51
1:B:300:THR:C	1:B:301:THR:C	2.78	0.50
1:B:417:PRO:HG3	2:B:433:GCP:C4	2.41	0.50
1:A:197:LEU:O	1:A:198:THR:C	2.52	0.50
1:B:61:ARG:HD3	3:B:546:HOH:O	2.10	0.50
1:B:292:LYS:HE3	1:B:293:GLN:OE1	2.11	0.50
1:B:300:THR:HG23	1:B:300:THR:O	2.09	0.50
1:B:300:THR:O	1:B:301:THR:C	2.54	0.50
1:A:375:MET:HE1	1:A:397:ASN:O	2.10	0.50
1:B:35:GLY:O	1:B:73:VAL:HG22	2.12	0.50
1:A:236:PRO:O	1:B:143:ARG:NH1	2.45	0.50
1:A:271:THR:CG2	1:A:307:THR:HG22	2.40	0.50
1:A:97:LEU:O	1:A:200:MET:HG2	2.12	0.50
1:A:281:GLU:OE1	1:A:306:ARG:HD2	2.12	0.50
1:B:380:GLU:H	1:B:380:GLU:CD	2.20	0.50
1:A:323:SER:HB3	1:B:258:TYR:CE2	2.47	0.49
1:A:317:ARG:O	1:A:320:GLN:HG2	2.13	0.49
1:A:411:ASP:HB3	1:A:426:ARG:HB3	1.93	0.49
1:B:44:VAL:O	1:B:46:ASN:N	2.45	0.49
1:B:274:GLY:O	1:B:306:ARG:NH2	2.45	0.49
1:B:358:THR:HB	1:B:365:TRP:CZ2	2.47	0.49
1:A:301:THR:HB	1:A:303:ARG:HH22	1.76	0.49
1:B:235:TYR:CD1	1:B:235:TYR:C	2.86	0.49
1:B:6:VAL:HG22	1:B:263:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:HD21	1:B:332:LEU:HB2	1.95	0.49
1:B:360:LEU:HD23	1:B:360:LEU:N	2.24	0.49
1:A:64:VAL:HG12	1:A:65:THR:N	2.27	0.49
1:A:304:ARG:NH1	1:A:304:ARG:HG3	2.27	0.49
1:B:399:ILE:HG23	1:B:410:ILE:HD12	1.95	0.49
1:B:418:ASP:CG	1:B:419:ARG:N	2.71	0.49
1:A:266:LEU:O	1:A:329:LEU:HA	2.13	0.49
1:B:267:LYS:C	1:B:269:TYR:N	2.69	0.49
1:A:46:ASN:ND2	3:A:541:HOH:O	2.46	0.49
1:A:56:PRO:CB	1:A:66:SER:HB3	2.42	0.49
1:A:238:VAL:HG23	1:B:143:ARG:HD2	1.95	0.49
1:A:113:LEU:O	1:A:117:ARG:HD2	2.13	0.48
1:A:13:ASP:OD2	1:A:305:ARG:CZ	2.61	0.48
1:A:393:GLN:O	1:A:397:ASN:ND2	2.46	0.48
1:A:310:LEU:HD23	1:A:343:LEU:HD21	1.95	0.48
1:A:196:ILE:HG22	1:A:197:LEU:HD23	1.94	0.48
1:B:62:GLU:H	1:B:62:GLU:HG3	1.42	0.48
1:A:97:LEU:HB3	1:A:200:MET:CE	2.43	0.48
1:B:409:PRO:HG3	1:B:426:ARG:HH12	1.78	0.48
1:A:291:CYS:SG	1:A:296:GLU:HB2	2.53	0.48
1:B:10:GLN:HG2	3:B:522:HOH:O	2.13	0.48
1:B:397:ASN:CG	1:B:400:LYS:NZ	2.70	0.48
1:A:111:VAL:HG22	1:A:131:ARG:HA	1.95	0.48
1:B:115:ASN:O	1:B:119:LYS:HG3	2.13	0.48
1:B:234:THR:HG21	1:B:277:PRO:CD	2.44	0.48
1:B:328:CYS:HA	1:B:412:ILE:O	2.14	0.48
1:B:268:ALA:HB2	1:B:332:LEU:HA	1.95	0.47
1:A:170:PHE:O	1:A:174:ASN:HB2	2.14	0.47
1:A:120:ALA:O	1:A:121:ARG:C	2.57	0.47
1:B:229:ASP:O	1:B:230:ILE:C	2.57	0.47
1:A:24:THR:HG22	1:A:24:THR:O	2.15	0.47
1:A:70:ASN:OD1	1:B:232:HIS:HE1	1.98	0.47
1:A:79:LEU:HD12	1:A:80:MET:HE2	1.95	0.47
1:A:358:THR:HG23	1:A:365:TRP:CZ2	2.49	0.47
1:A:412:ILE:HG12	1:A:424:ILE:HG12	1.95	0.47
1:B:263:LEU:HD11	1:B:328:CYS:HB2	1.96	0.47
1:A:132:GLY:C	1:A:135:PRO:HD2	2.40	0.47
1:B:360:LEU:O	1:B:362:ALA:N	2.48	0.47
1:A:280:THR:HG22	1:A:372:TYR:CZ	2.49	0.47
1:B:363:ASP:HB2	3:B:516:HOH:O	2.14	0.47
1:A:64:VAL:CG1	1:A:65:THR:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HB3	1:B:179:GLU:O	2.15	0.47
1:B:360:LEU:O	1:B:361:ALA:C	2.57	0.46
1:B:303:ARG:O	1:B:304:ARG:C	2.59	0.46
1:B:279:PRO:O	1:B:370:PRO:HG3	2.16	0.46
1:A:79:LEU:HD12	1:A:80:MET:CE	2.46	0.46
1:A:348:ARG:HG2	1:A:348:ARG:NH1	2.30	0.46
1:B:14:GLU:HB3	1:B:265:ILE:HG22	1.97	0.46
1:A:46:ASN:HB2	1:A:89:ARG:HG3	1.97	0.46
1:A:171:GLN:O	1:A:175:TYR:HB3	2.15	0.46
1:B:210:GLN:O	1:B:214:ARG:HB2	2.16	0.46
1:A:311:ASP:OD1	1:A:311:ASP:C	2.57	0.46
1:A:61:ARG:HD2	1:A:61:ARG:N	2.29	0.46
1:A:299:ALA:O	1:A:300:THR:HB	2.16	0.46
1:A:349:MET:SD	1:A:368:VAL:CG1	2.99	0.46
1:A:360:LEU:O	1:A:362:ALA:N	2.43	0.46
1:A:170:PHE:CD1	1:A:170:PHE:C	2.94	0.46
1:B:273:VAL:CG2	1:B:305:ARG:HG2	2.45	0.46
1:B:326:GLY:HA2	1:B:408:VAL:CG1	2.46	0.45
1:B:388:ARG:HD3	1:B:425:LEU:HD21	1.98	0.45
1:B:396:LEU:O	1:B:400:LYS:HG2	2.16	0.45
1:B:271:THR:HG21	1:B:296:GLU:HG3	1.98	0.45
1:A:294:GLY:O	1:A:295:ASN:HB3	2.16	0.45
1:A:165:MET:SD	1:A:183:TYR:HA	2.57	0.45
1:B:388:ARG:HD3	1:B:425:LEU:CD2	2.46	0.45
1:B:418:ASP:OD2	1:B:421:GLU:HG3	2.16	0.45
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.82	0.45
1:B:81:LYS:HE2	1:B:81:LYS:HB3	1.89	0.45
1:B:315:VAL:O	1:B:319:VAL:HG23	2.16	0.45
1:A:266:LEU:O	1:A:329:LEU:HD12	2.16	0.45
1:B:267:LYS:O	1:B:269:TYR:N	2.50	0.45
1:A:280:THR:HG22	1:A:372:TYR:OH	2.16	0.45
1:A:280:THR:O	1:A:308:GLY:HA3	2.16	0.45
1:A:400:LYS:O	1:A:404:GLU:HG3	2.17	0.45
1:B:45:ILE:N	1:B:48:GLU:O	2.51	0.44
1:A:79:LEU:HD13	1:A:79:LEU:O	2.16	0.44
1:B:300:THR:O	1:B:300:THR:CG2	2.65	0.44
1:B:329:LEU:HD21	1:B:332:LEU:HD13	1.98	0.44
1:B:39:ALA:HB3	1:B:53:HIS:HA	1.99	0.44
1:A:19:ILE:H	1:A:19:ILE:CD1	2.28	0.44
1:A:101:GLU:HG2	3:A:439:HOH:O	2.17	0.44
1:B:38:ASN:O	1:B:39:ALA:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:MET:HE1	1:B:94:ARG:HD2	1.99	0.44
1:A:314:ALA:O	1:A:317:ARG:HB3	2.17	0.44
1:B:214:ARG:HH11	1:B:214:ARG:HD2	1.65	0.44
1:A:53:HIS:N	1:A:82:GLU:OE2	2.48	0.44
1:A:384:GLY:CA	1:A:421:GLU:HG3	2.40	0.44
1:B:265:ILE:HG13	1:B:328:CYS:HB3	1.99	0.44
1:A:107:LEU:H	1:A:110:HIS:HD2	1.65	0.44
1:A:424:ILE:N	3:A:534:HOH:O	2.50	0.44
1:A:426:ARG:O	1:A:427:ASP:CB	2.57	0.43
1:A:66:SER:O	1:A:97:LEU:HD12	2.18	0.43
1:B:109:TYR:O	1:B:113:LEU:HG	2.18	0.43
1:B:282:LEU:HD21	1:B:309:TRP:CD1	2.53	0.43
1:B:385:VAL:HG11	1:B:391:LEU:HD13	2.01	0.43
1:A:386:LYS:HD3	1:A:420:THR:O	2.18	0.43
1:B:212:ARG:O	1:B:213:GLN:C	2.62	0.43
1:B:214:ARG:NH2	3:B:573:HOH:O	2.51	0.43
1:A:345:VAL:O	1:A:346:ALA:CB	2.66	0.43
1:B:79:LEU:O	1:B:83:MET:HG3	2.18	0.43
1:B:302:GLY:O	1:B:304:ARG:N	2.51	0.43
1:A:16:LYS:O	1:A:20:VAL:HG23	2.18	0.43
1:B:195:ASP:O	1:B:199:SER:HB3	2.19	0.43
1:A:160:LYS:O	1:A:161:LEU:C	2.62	0.43
1:A:337:GLY:H	1:A:379:SER:HA	1.84	0.43
1:B:183:TYR:HB2	3:B:454:HOH:O	2.19	0.43
1:B:397:ASN:HA	1:B:400:LYS:HZ2	1.83	0.43
1:A:113:LEU:HD11	1:A:171:GLN:OE1	2.19	0.43
1:A:83:MET:HG2	1:A:93:VAL:HG11	2.01	0.43
1:B:70:ASN:CB	1:B:102:ALA:HB3	2.48	0.43
1:B:342:LYS:HG2	1:B:374:THR:OG1	2.19	0.43
1:A:79:LEU:HD13	1:A:79:LEU:C	2.44	0.42
1:A:80:MET:HE1	1:A:83:MET:SD	2.59	0.42
1:A:291:CYS:SG	1:A:304:ARG:NH1	2.78	0.42
1:A:311:ASP:O	1:A:315:VAL:HG23	2.19	0.42
1:B:17:GLY:N	2:B:433:GCP:O1A	2.51	0.42
1:B:129:THR:HA	1:B:131:ARG:NH2	2.34	0.42
1:A:6:VAL:O	1:A:7:LEU:HB3	2.18	0.42
1:A:107:LEU:O	1:A:110:HIS:HB2	2.19	0.42
1:B:6:VAL:HG13	1:B:265:ILE:HD11	2.00	0.42
1:B:349:MET:HG3	1:B:353:ARG:CZ	2.49	0.42
1:A:86:LEU:HB3	1:A:91:ILE:HB	2.00	0.42
1:B:6:VAL:HG13	1:B:265:ILE:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:HD3	3:A:549:HOH:O	2.19	0.42
1:A:97:LEU:HD23	1:A:200:MET:HE1	1.97	0.42
1:A:312:THR:HB	1:A:344:CYS:O	2.20	0.42
1:A:333:ASP:HB2	1:A:383:PHE:HD1	1.84	0.42
1:B:129:THR:HA	1:B:131:ARG:HH12	1.78	0.42
1:B:110:HIS:HE1	1:B:139:ASP:OD2	2.02	0.42
1:A:79:LEU:HD11	1:A:83:MET:SD	2.59	0.42
1:B:76:PRO:O	1:B:77:ALA:C	2.62	0.42
1:A:335:LEU:O	1:A:338:LEU:HB2	2.19	0.42
1:A:345:VAL:HG12	1:A:405:LEU:CD1	2.48	0.42
1:B:28:LYS:O	1:B:28:LYS:NZ	2.43	0.42
1:B:229:ASP:O	1:B:231:ASP:N	2.53	0.42
1:B:427:ASP:HA	1:B:428:PRO:HD3	1.77	0.42
1:B:298:GLY:HA3	3:B:566:HOH:O	2.20	0.42
1:B:304:ARG:NE	3:B:518:HOH:O	2.51	0.42
1:A:83:MET:O	1:A:84:LYS:C	2.61	0.42
1:A:298:GLY:O	1:A:299:ALA:HB3	2.20	0.42
1:B:91:ILE:O	1:B:93:VAL:N	2.52	0.42
1:A:227:LEU:HA	1:A:227:LEU:HD23	1.81	0.41
1:A:299:ALA:O	1:A:300:THR:CB	2.68	0.41
1:B:33:TYR:CE2	1:B:221:GLU:C	2.98	0.41
1:B:73:VAL:O	1:B:73:VAL:HG23	2.20	0.41
1:B:267:LYS:O	1:B:268:ALA:C	2.63	0.41
1:B:303:ARG:HH11	1:B:303:ARG:HD3	1.68	0.41
1:B:347:TYR:HB3	1:B:368:VAL:HG13	2.02	0.41
1:A:142:ALA:O	1:A:143:ARG:HB2	2.18	0.41
1:A:170:PHE:HA	3:A:527:HOH:O	2.19	0.41
1:A:203:ASP:HB3	3:A:441:HOH:O	2.19	0.41
1:A:267:LYS:HD2	1:A:331:LYS:HD2	2.01	0.41
1:A:336:ASP:O	1:A:337:GLY:C	2.62	0.41
1:B:134:GLY:O	1:B:138:GLU:HG3	2.20	0.41
1:B:232:HIS:HB2	1:B:321:LEU:HD11	2.02	0.41
1:B:316:ARG:HE	1:B:316:ARG:HB2	1.60	0.41
1:B:388:ARG:NH1	1:B:425:LEU:HD22	2.31	0.41
1:A:59:ILE:HG21	1:A:86:LEU:CD1	2.50	0.41
1:B:37:HIS:HA	1:B:53:HIS:O	2.20	0.41
1:A:349:MET:HE1	1:A:359:PRO:HB3	2.02	0.41
1:B:73:VAL:HB	1:B:106:ILE:HD11	2.02	0.41
1:B:304:ARG:CZ	3:B:518:HOH:O	2.68	0.41
1:B:277:PRO:HA	3:B:455:HOH:O	2.20	0.41
1:A:289:PHE:CE1	1:A:338:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD13	1:A:341:VAL:CG1	2.48	0.41
1:A:361:ALA:N	1:B:101:GLU:OE2	2.53	0.41
1:A:94:ARG:HH11	1:A:94:ARG:HD2	1.71	0.41
1:B:83:MET:CE	1:B:94:ARG:HD2	2.51	0.41
1:A:235:TYR:CG	1:A:236:PRO:HA	2.55	0.41
1:A:427:ASP:HA	1:A:428:PRO:HD3	1.88	0.41
1:B:2:ASN:ND2	1:B:215:GLY:O	2.53	0.41
1:B:267:LYS:C	1:B:269:TYR:H	2.29	0.41
1:A:214:ARG:HH11	1:A:214:ARG:HD2	1.66	0.41
1:A:342:LYS:HE2	1:A:374:THR:OG1	2.21	0.41
1:B:124:LYS:O	1:B:125:ALA:HB2	2.21	0.41
1:B:361:ALA:HB2	3:B:533:HOH:O	2.21	0.40
1:B:268:ALA:CB	1:B:332:LEU:HA	2.51	0.40
1:B:347:TYR:HB3	1:B:349:MET:CE	2.51	0.40
1:A:32:ARG:NH1	1:A:39:ALA:HB2	2.36	0.40
1:B:131:ARG:HG3	1:B:133:ILE:H	1.86	0.40
1:A:97:LEU:HD23	1:A:200:MET:HE2	2.04	0.40
1:A:137:TYR:O	1:A:140:LYS:HB3	2.21	0.40
1:A:385:VAL:HG12	1:A:423:MET:HE2	2.03	0.40
1:A:403:GLU:HG2	1:A:409:PRO:HA	2.02	0.40
1:A:407:GLY:O	1:A:408:VAL:HG23	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	429/431 (100%)	372 (87%)	41 (10%)	16 (4%)	2	1
1	B	429/431 (100%)	366 (85%)	44 (10%)	19 (4%)	2	1
All	All	858/862 (100%)	738 (86%)	85 (10%)	35 (4%)	2	1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	THR
1	B	39	ALA
1	B	45	ILE
1	B	125	ALA
1	B	235	TYR
1	B	300	THR
1	B	361	ALA
1	B	364	ASP
1	A	120	ALA
1	A	121	ARG
1	A	230	ILE
1	B	2	ASN
1	B	108	ASP
1	B	130	GLY
1	B	362	ALA
1	A	38	ASN
1	A	128	THR
1	A	303	ARG
1	A	346	ALA
1	B	40	GLY
1	B	268	ALA
1	B	304	ARG
1	A	127	GLY
1	A	194	ALA
1	A	362	ALA
1	A	427	ASP
1	A	46	ASN
1	B	126	ILE
1	B	255	GLY
1	B	360	LEU
1	B	230	ILE
1	B	427	ASP
1	A	20	VAL
1	A	45	ILE
1	A	132	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	353/353 (100%)	318 (90%)	35 (10%)	7	9
1	B	353/353 (100%)	317 (90%)	36 (10%)	7	8
All	All	706/706 (100%)	635 (90%)	71 (10%)	7	9

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	31	VAL
1	A	34	GLN
1	A	38	ASN
1	A	43	LEU
1	A	44	VAL
1	A	45	ILE
1	A	61	ARG
1	A	81	LYS
1	A	85	GLU
1	A	89	ARG
1	A	99	LEU
1	A	101	GLU
1	A	128	THR
1	A	131	ARG
1	A	138	GLU
1	A	155	GLU
1	A	156	THR
1	A	164	VAL
1	A	165	MET
1	A	190	THR
1	A	196	ILE
1	A	198	THR
1	A	202	VAL
1	A	207	LEU
1	A	239	THR
1	A	240	SER
1	A	270	SER
1	A	273	VAL
1	A	284	ASP
1	A	333	ASP
1	A	355	VAL
1	A	357	THR

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Mol	Chain	Res	Type
1	A	379	SER
1	A	386	LYS
1	B	2	ASN
1	B	7	LEU
1	B	28	LYS
1	B	34	GLN
1	B	37	HIS
1	B	50	THR
1	B	62	GLU
1	B	84	LYS
1	B	126	ILE
1	B	135	PRO
1	B	148	VAL
1	B	173	VAL
1	B	179	GLU
1	B	193	VAL
1	B	202	VAL
1	B	205	SER
1	B	207	LEU
1	B	213	GLN
1	B	234	THR
1	B	240	SER
1	B	254	LEU
1	B	270	SER
1	B	295	ASN
1	B	312	THR
1	B	329	LEU
1	B	341	VAL
1	B	343	LEU
1	B	355	VAL
1	B	360	LEU
1	B	375	MET
1	B	391	LEU
1	B	413	ILE
1	B	415	THR
1	B	418	ASP
1	B	420	THR
1	B	422	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	41	HIS
1	A	110	HIS
1	A	393	GLN
1	B	2	ASN
1	B	37	HIS
1	B	41	HIS
1	B	53	HIS
1	B	110	HIS
1	B	184	GLN
1	B	213	GLN
1	B	232	HIS
1	B	242	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	GCP	B	433	-	32,34,34	1.72	7 (21%)	49,54,54	1.90	13 (26%)
2	GCP	A	432	-	32,34,34	1.74	7 (21%)	49,54,54	1.51	9 (18%)

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	GCP	B	433	-	-	2/19/38/38	0/3/3/3
2	GCP	A	432	-	-	9/19/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	433	GCP	PA-O3A	4.44	1.64	1.59
2	A	432	GCP	PA-O3A	4.22	1.64	1.59
2	A	432	GCP	PB-O3A	4.09	1.63	1.58
2	B	433	GCP	PB-O3A	3.94	1.62	1.58
2	B	433	GCP	PB-O2B	-3.71	1.47	1.56
2	A	432	GCP	PB-O2B	-3.59	1.47	1.56
2	A	432	GCP	C2'-C3'	3.33	1.62	1.53
2	A	432	GCP	C1'-N9	-3.20	1.38	1.47
2	B	433	GCP	C1'-N9	-2.96	1.39	1.47
2	B	433	GCP	PG-O2G	-2.74	1.48	1.55
2	B	433	GCP	PG-O3G	-2.56	1.49	1.55
2	A	432	GCP	PG-O3G	-2.31	1.49	1.55
2	B	433	GCP	C4-N3	2.19	1.39	1.34
2	A	432	GCP	O4'-C1'	2.19	1.47	1.42

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	433	GCP	O4'-C1'-C2'	-5.69	94.45	106.62
2	A	432	GCP	O1G-PG-C3B	-4.59	101.36	111.37
2	B	433	GCP	C2'-C1'-N9	3.88	124.05	113.25
2	B	433	GCP	O4'-C1'-N9	-3.65	100.09	108.36
2	B	433	GCP	O2'-C2'-C3'	-3.62	100.20	111.82
2	A	432	GCP	N9-C8-N7	3.47	119.84	113.40
2	B	433	GCP	C3'-C2'-C1'	3.38	107.86	101.46
2	A	432	GCP	C8-N7-C5	-3.33	98.33	104.26
2	B	433	GCP	N9-C8-N7	2.88	118.75	113.40
2	B	433	GCP	O2B-PB-O1B	2.51	118.11	109.95
2	B	433	GCP	O5'-PA-O1A	-2.48	99.10	108.94
2	B	433	GCP	O3G-PG-O2G	2.44	114.92	107.96
2	A	432	GCP	O2G-PG-C3B	2.43	112.30	106.40
2	A	432	GCP	O3G-PG-C3B	-2.42	100.52	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	433	GCP	O3'-C3'-C2'	2.39	119.48	111.82
2	B	433	GCP	C5-C4-N3	-2.37	124.62	128.39
2	A	432	GCP	C8-N9-C4	-2.23	101.85	106.03
2	B	433	GCP	C2-N3-C4	2.21	116.10	112.30
2	A	432	GCP	O4'-C4'-C5'	-2.20	102.28	109.33
2	B	433	GCP	O3G-PG-C3B	-2.18	101.12	106.40
2	A	432	GCP	O2'-C2'-C3'	2.06	118.41	111.82
2	A	432	GCP	O3G-PG-O2G	2.01	113.68	107.96

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	432	GCP	PB-C3B-PG-O2G
2	A	432	GCP	PG-C3B-PB-O3A
2	A	432	GCP	PB-O3A-PA-O5'
2	A	432	GCP	C5'-O5'-PA-O3A
2	A	432	GCP	C5'-O5'-PA-O1A
2	A	432	GCP	C5'-O5'-PA-O2A
2	A	432	GCP	PB-C3B-PG-O3G
2	B	433	GCP	C5'-O5'-PA-O3A
2	A	432	GCP	C4'-C5'-O5'-PA
2	A	432	GCP	PB-C3B-PG-O1G
2	B	433	GCP	PB-O3A-PA-O2A

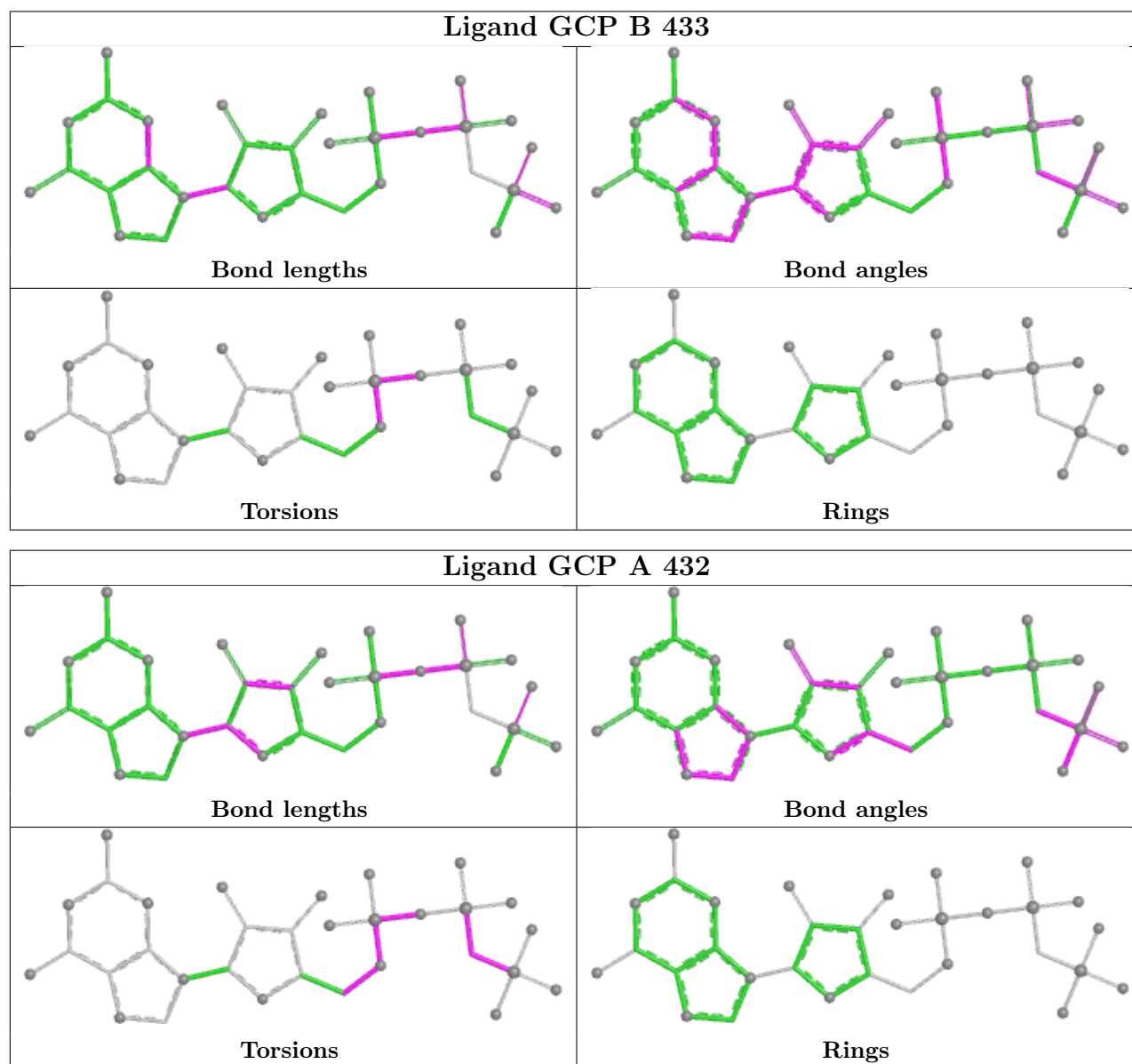
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	433	GCP	3	0
2	A	432	GCP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

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Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	126:ILE	C	127:GLY	N	1.70
1	B	300:THR	C	301:THR	N	1.68
1	A	130:GLY	C	131:ARG	N	1.62

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	431/431 (100%)	-0.27	8 (1%) 66 68	9, 23, 49, 68	0
1	B	431/431 (100%)	-0.46	1 (0%) 91 91	7, 19, 41, 61	0
All	All	862/862 (100%)	-0.36	9 (1%) 79 80	7, 21, 46, 68	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	THR	5.2
1	A	127	GLY	4.4
1	B	125	ALA	4.1
1	A	128	THR	3.8
1	A	118	GLU	2.2
1	A	361	ALA	2.2
1	A	122	GLY	2.1
1	A	298	GLY	2.1
1	A	123	ALA	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 oligosaccharides in this entry.

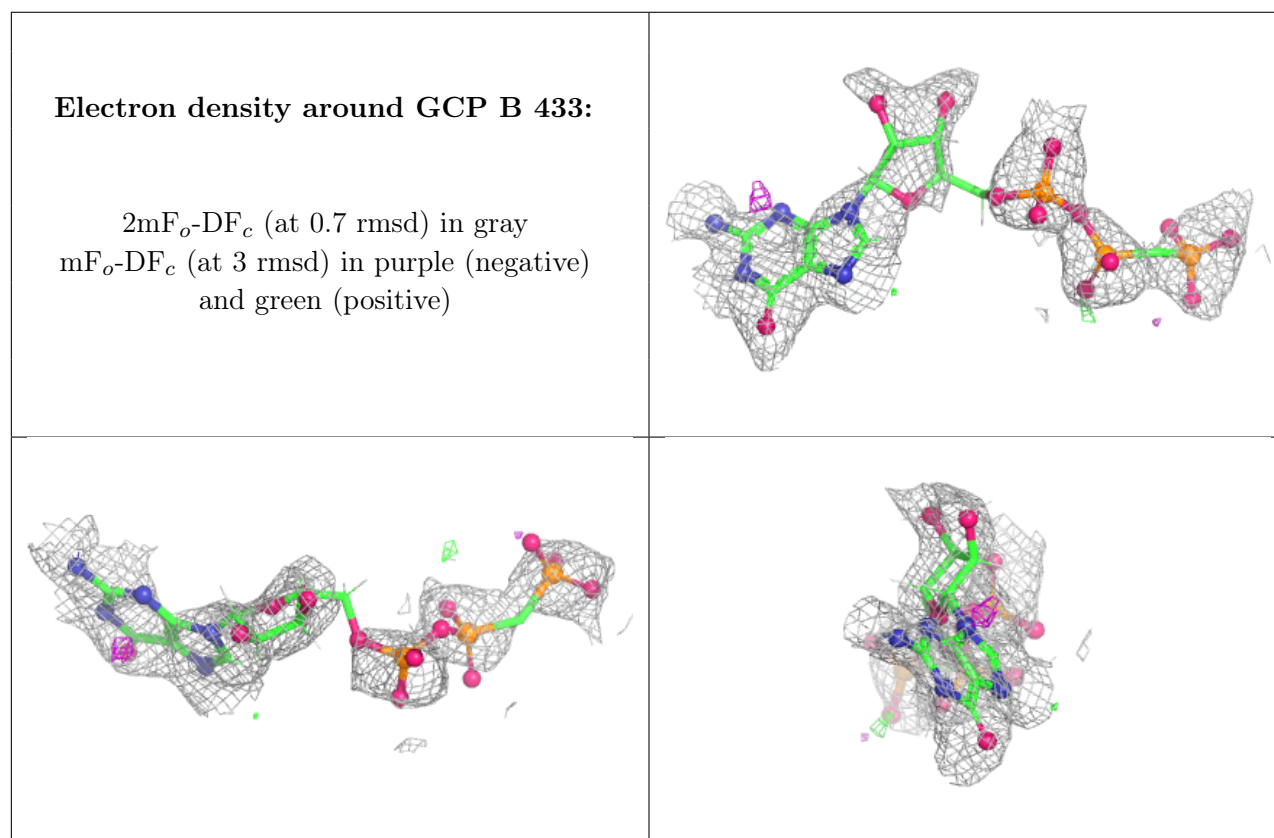
6.4 Ligands [i](#)

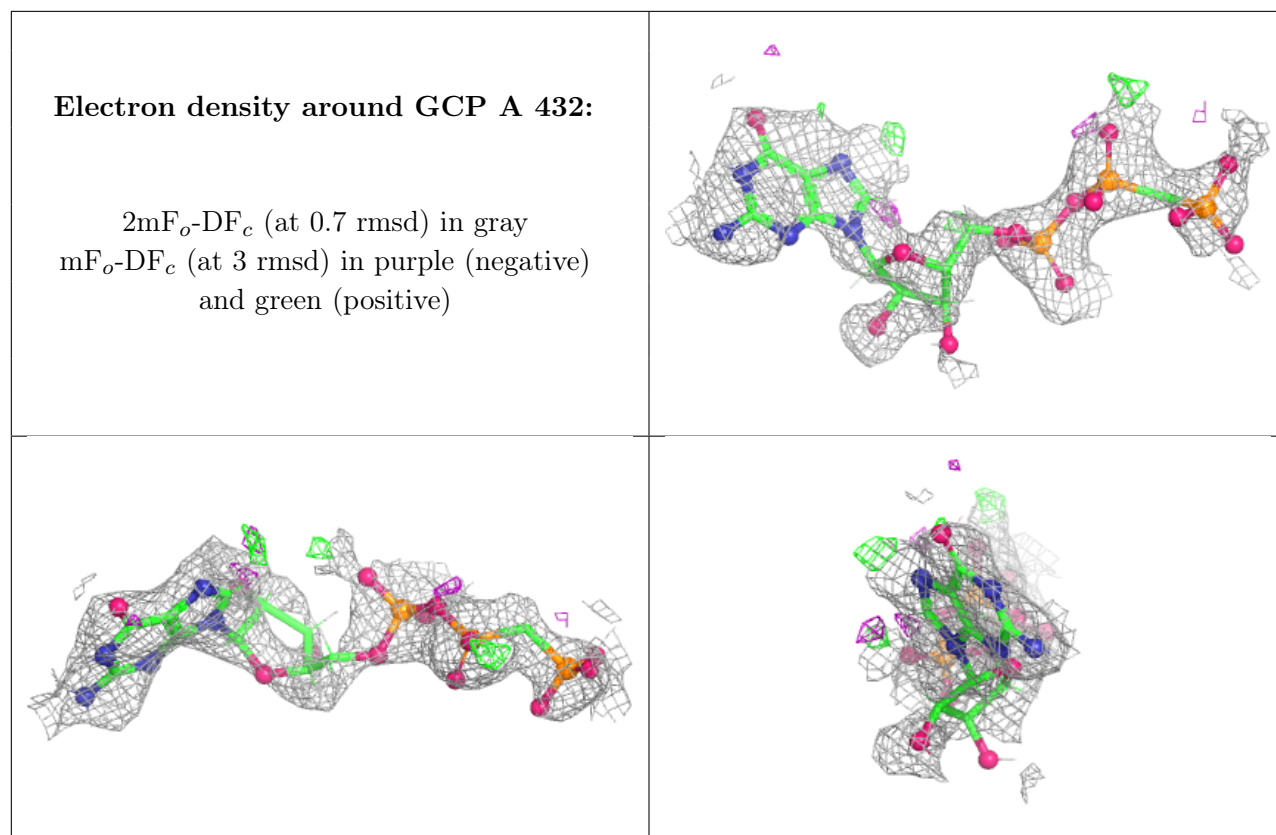
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
2	GCP	B	433	32/32	0.87	0.10	0,53,58,59	0
2	GCP	A	432	32/32	0.90	0.08	0,42,53,54	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.