



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:16 PM UTC

PDB ID : 1HON / pdb_00001hon
Title : STRUCTURE OF GUANINE NUCLEOTIDE (GPPCP) COMPLEX OF
ADENYLOSUCCINATE SYNTHETASE FROM ESCHERICHIA COLI AT
PH 6.5 AND 25 DEGREE CELSIUS
Authors : Poland, B.W.; Hou, Z.; Bruns, C.; Fromm, H.J.; Honzatko, R.B.
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

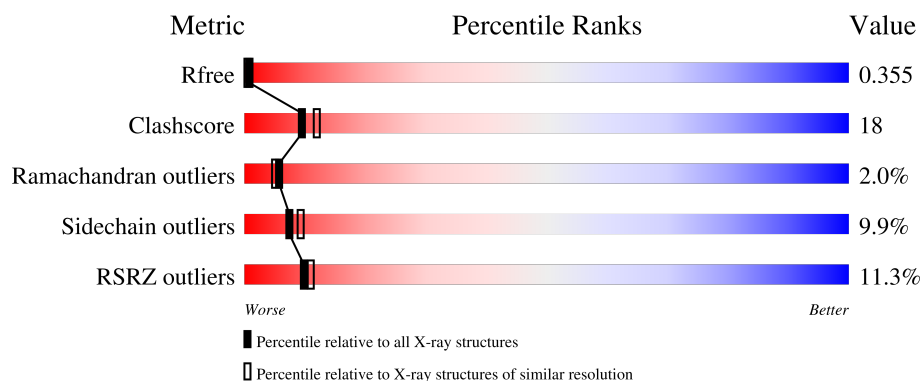
1 Overall quality at a glance

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	15% 54% 37% 8%
1	B	431	7% 63% 33% • •

2 Entry composition [i](#)

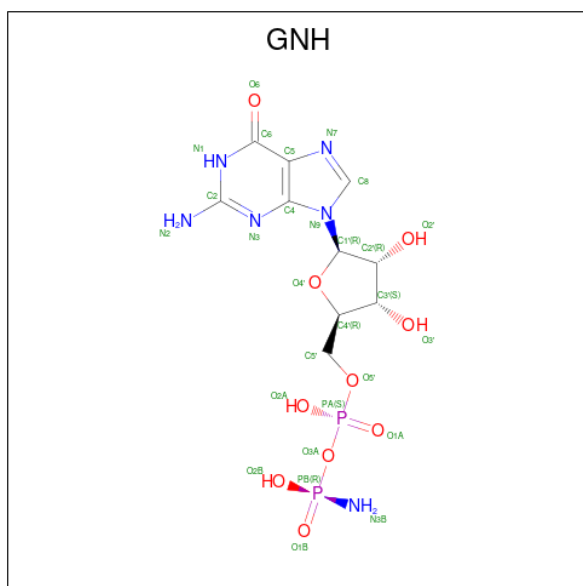
There are 3 unique types of molecules in this entry. The entry contains 9338 atoms, of which 2282 are hydrogens and 0 are deuteriums.

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 AMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNH) (formula: $C_{10}H_{16}N_6O_{10}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			42	10	14	6	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	195	Total	H	O	0	0
			585	390	195		

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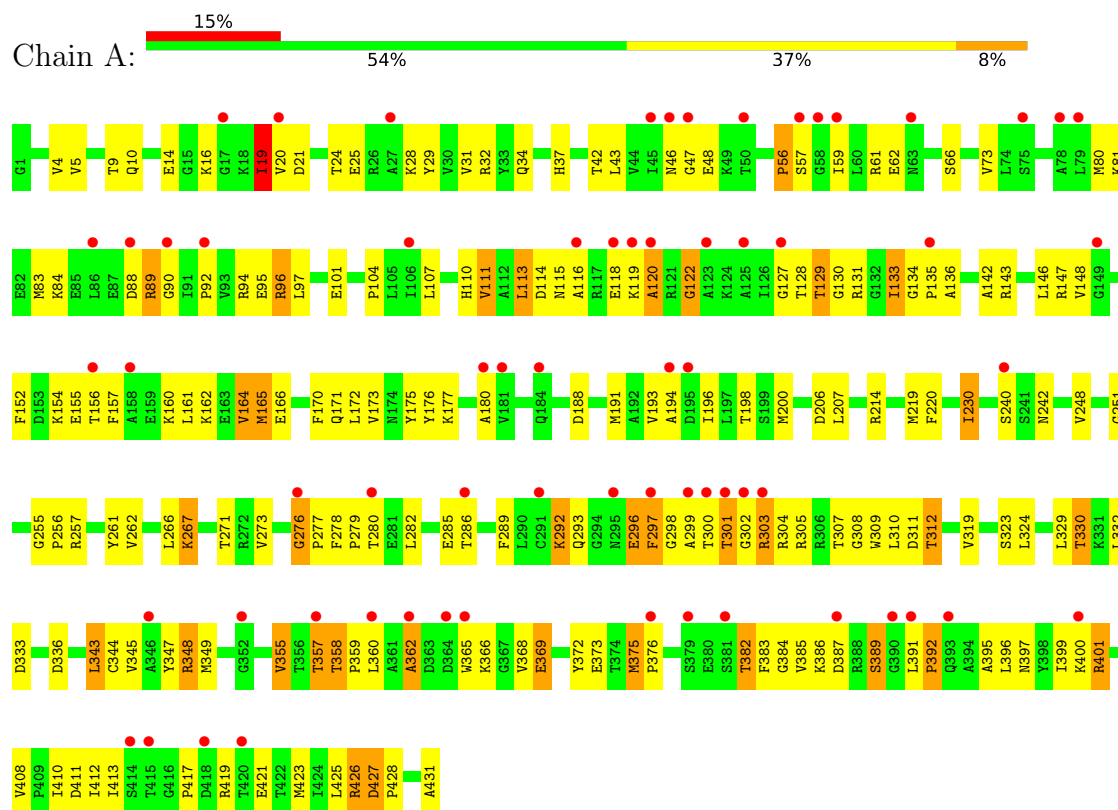
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	191	Total	H	O	0	0
			573	382	191		

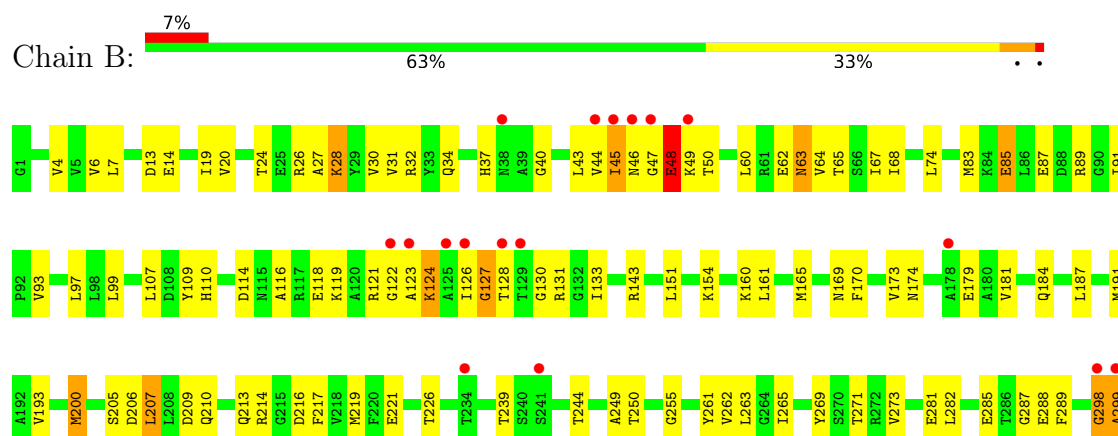
3 Residue-property plots

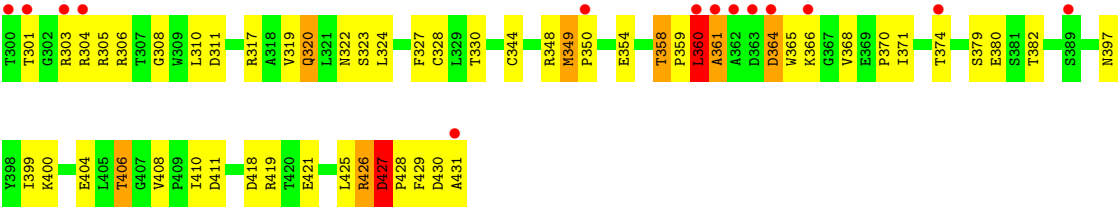
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	72.60Å 92.91Å 119.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 15.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 72.5 (15.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.27Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , 0.230 0.306 , 0.355	Depositor DCC
R_{free} test set	2670 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	9338	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows:

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: GNH

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	0.90	2/3379 (0.1%)	1.17	16/4577 (0.3%)
1	B	0.63	0/3379	1.04	11/4577 (0.2%)
All	All	0.77	2/6758 (0.0%)	1.11	27/9154 (0.3%)

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	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	VAL	CA-CB	5.91	1.61	1.54
1	A	19	ILE	CA-CB	5.24	1.60	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	LEU	O-C-N	-21.85	93.53	122.59
1	B	427	ASP	CA-C-N	7.74	128.45	119.47
1	B	427	ASP	C-N-CA	7.74	128.45	119.47
1	A	375	MET	CA-C-N	7.09	127.06	119.76
1	A	375	MET	C-N-CA	7.09	127.06	119.76
1	A	31	VAL	N-CA-C	7.00	117.97	108.17
1	A	427	ASP	CA-C-N	6.51	127.02	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	ASP	C-N-CA	6.51	127.02	119.47
1	A	278	PHE	CA-C-N	6.50	127.96	119.84
1	A	278	PHE	C-N-CA	6.50	127.96	119.84
1	B	31	VAL	N-CA-C	6.29	116.91	108.11
1	B	287	GLY	N-CA-C	-6.20	105.27	112.83
1	B	91	ILE	CB-CA-C	-6.18	105.19	110.94
1	B	370	PRO	N-CA-C	5.93	119.93	110.21
1	A	134	GLY	CA-C-N	-5.61	113.11	119.28
1	A	134	GLY	C-N-CA	-5.61	113.11	119.28
1	A	47	GLY	N-CA-C	-5.54	106.86	114.67
1	B	74	LEU	N-CA-C	5.45	117.61	108.73
1	A	251	GLY	N-CA-C	5.38	120.59	114.67
1	A	389	SER	N-CA-C	-5.36	106.05	113.18
1	B	93	VAL	N-CA-C	5.35	115.98	110.36
1	A	358	THR	CA-C-N	-5.21	114.34	119.92
1	A	358	THR	C-N-CA	-5.21	114.34	119.92
1	A	345	VAL	CB-CA-C	-5.17	105.59	110.65
1	B	349	MET	CA-C-N	5.17	126.30	119.84
1	B	349	MET	C-N-CA	5.17	126.30	119.84
1	A	276	GLY	O-C-N	-5.01	116.76	121.77

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	GLY	Mainchain
1	A	296	GLU	Mainchain
1	B	360	LEU	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	3326	142	5
1	B	3321	748	3326	105	2
2	A	28	14	14	1	0
3	A	195	390	0	9	6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	191	382	0	6	5
All	All	7056	2282	6666	239	12

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 18.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HG13	1:A:219:MET:HE1	1.40	1.03
1:A:118:GLU:HB2	1:A:129:THR:H	1.25	0.98
1:A:80:MET:HE2	1:A:193:VAL:HG11	1.51	0.93
1:A:94:ARG:HA	1:A:200:MET:HE2	1.54	0.90
1:B:43:LEU:HD22	1:B:47:GLY:HA3	1.57	0.86
1:A:92:PRO:HB2	1:A:95:GLU:HG2	1.59	0.84
1:A:256:PRO:HD2	1:B:323:SER:OG	1.78	0.84
1:B:304:ARG:NH1	1:B:304:ARG:HA	1.93	0.84
1:A:42:THR:HG22	2:A:432:GNH:O2B	1.78	0.83
1:A:21:ASP:HB3	1:A:419:ARG:NH2	1.94	0.83
1:A:273:VAL:HA	1:A:304:ARG:O	1.82	0.79
1:B:327:PHE:HE2	1:B:406:THR:HG21	1.50	0.76
1:A:118:GLU:HB2	1:A:129:THR:N	2.02	0.75
1:A:301:THR:H	1:A:305:ARG:HH22	1.34	0.74
1:A:25:GLU:HG2	1:A:61:ARG:CZ	2.19	0.73
1:A:156:THR:O	1:A:160:LYS:HG3	1.88	0.72
1:A:312:THR:HB	1:A:344:CYS:O	1.89	0.72
1:B:114:ASP:HB3	1:B:130:GLY:HA2	1.72	0.72
1:A:277:PRO:HB3	1:A:365:TRP:HB3	1.72	0.71
1:B:20:VAL:HG13	1:B:219:MET:HE1	1.73	0.70
1:B:226:THR:HG23	1:B:244:THR:HG22	1.73	0.70
1:B:349:MET:HE1	1:B:359:PRO:HG3	1.74	0.69
1:A:24:THR:HG22	1:A:61:ARG:HE	1.56	0.69
1:A:118:GLU:HB3	1:A:129:THR:OG1	1.93	0.69
1:A:296:GLU:HB3	1:A:305:ARG:HD2	1.75	0.68
1:A:397:ASN:HA	1:A:400:LYS:HZ3	1.60	0.67
1:A:25:GLU:HG2	1:A:61:ARG:NH2	2.09	0.67
1:B:349:MET:SD	1:B:368:VAL:HG12	2.35	0.67
1:A:80:MET:HE2	1:A:193:VAL:CG1	2.24	0.66
1:A:319:VAL:HA	1:A:324:LEU:HD12	1.79	0.65
1:A:19:ILE:N	1:A:19:ILE:HD13	2.11	0.65
1:B:298:GLY:HA3	1:B:305:ARG:CZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG22	1:B:305:ARG:HG2	1.80	0.64
1:A:162:LYS:O	1:A:166:GLU:HG3	1.98	0.64
1:A:118:GLU:HG2	1:A:127:GLY:CA	2.28	0.63
1:B:206:ASP:O	1:B:210:GLN:HG2	1.98	0.63
1:A:14:GLU:O	1:A:330:THR:HG21	1.99	0.63
1:A:280:THR:HG23	1:A:372:TYR:OH	1.98	0.63
1:A:426:ARG:HD3	1:A:431:ALA:HB2	1.81	0.62
1:A:118:GLU:HG2	1:A:127:GLY:HA3	1.82	0.62
1:A:21:ASP:HB3	1:A:419:ARG:HH21	1.64	0.61
1:A:114:ASP:OD1	1:A:128:THR:HG22	2.00	0.61
1:B:97:LEU:HD23	1:B:200:MET:CE	2.30	0.61
1:B:400:LYS:O	1:B:404:GLU:HG3	2.00	0.61
1:A:271:THR:HG22	1:A:307:THR:HG22	1.82	0.61
1:A:16:LYS:HE3	3:A:559:HOH:O	2.01	0.61
1:A:92:PRO:HB2	1:A:95:GLU:CG	2.31	0.60
1:B:28:LYS:O	1:B:28:LYS:HD3	2.01	0.60
1:B:304:ARG:HA	1:B:304:ARG:CZ	2.31	0.60
1:A:94:ARG:HA	1:A:200:MET:CE	2.30	0.60
1:A:280:THR:HG22	1:A:309:TRP:H	1.68	0.59
1:A:176:TYR:O	1:A:177:LYS:HB2	2.02	0.59
1:A:280:THR:HG22	1:A:280:THR:O	2.02	0.59
1:A:66:SER:O	1:A:97:LEU:HD12	2.03	0.59
1:A:365:TRP:O	1:A:368:VAL:HG22	2.01	0.59
1:A:329:LEU:HD21	1:A:332:LEU:HD13	1.86	0.58
1:A:24:THR:CG2	1:A:61:ARG:HG3	2.33	0.58
1:B:107:LEU:H	1:B:110:HIS:HD2	1.51	0.58
1:B:14:GLU:HB3	1:B:265:ILE:HG22	1.84	0.58
1:A:152:PHE:CE1	1:A:198:THR:HB	2.38	0.58
1:A:131:ARG:HG2	1:A:131:ARG:HH11	1.70	0.57
1:A:172:LEU:HA	1:A:176:TYR:HB2	1.86	0.57
1:B:399:ILE:HG23	1:B:410:ILE:HD12	1.86	0.57
1:A:366:LYS:HG3	3:A:463:HOH:O	2.02	0.57
1:A:131:ARG:HG2	1:A:131:ARG:NH1	2.19	0.57
1:B:37:HIS:CE1	1:B:131:ARG:HG3	2.40	0.57
1:B:28:LYS:HD3	1:B:28:LYS:C	2.30	0.56
1:B:285:GLU:HA	1:B:288:GLU:HB2	1.87	0.56
1:A:24:THR:HG22	1:A:61:ARG:HG3	1.87	0.56
1:A:73:VAL:HG21	1:A:133:ILE:HG12	1.87	0.56
1:A:426:ARG:NH1	1:A:426:ARG:HG3	2.20	0.56
1:A:426:ARG:HH11	1:A:426:ARG:CG	2.19	0.56
1:A:32:ARG:HG2	1:A:56:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:THR:HA	1:B:306:ARG:O	2.06	0.56
1:A:348:ARG:HB3	1:A:369:GLU:HB3	1.88	0.56
1:B:216:ASP:HA	3:B:579:HOH:O	2.05	0.55
1:A:323:SER:HB3	1:B:255:GLY:HA3	1.88	0.55
1:A:160:LYS:O	1:A:164:VAL:HG23	2.07	0.55
1:A:142:ALA:O	1:A:143:ARG:HB2	2.07	0.55
1:A:170:PHE:HZ	1:B:174:ASN:O	1.90	0.55
1:B:298:GLY:HA3	1:B:305:ARG:NH2	2.22	0.55
1:A:131:ARG:HA	3:A:481:HOH:O	2.07	0.55
1:A:193:VAL:O	1:A:194:ALA:C	2.47	0.55
1:A:242:ASN:ND2	1:B:250:THR:HG23	2.22	0.54
1:A:343:LEU:HD11	1:A:401:ARG:HB3	1.89	0.54
1:B:27:ALA:O	1:B:64:VAL:HG22	2.07	0.54
1:A:28:LYS:HE2	1:A:29:TYR:CZ	2.42	0.54
1:A:329:LEU:HB2	1:A:410:ILE:HD13	1.89	0.54
1:B:109:TYR:HA	1:B:181:VAL:HG21	1.90	0.54
1:B:299:ALA:HB1	1:B:303:ARG:HG3	1.89	0.53
1:A:298:GLY:HA3	1:A:302:GLY:O	2.09	0.53
1:B:45:ILE:O	1:B:46:ASN:HB2	2.08	0.53
1:A:347:TYR:HD2	1:A:359:PRO:HD3	1.74	0.53
1:B:97:LEU:HD23	1:B:200:MET:HE2	1.90	0.53
1:B:43:LEU:HB3	1:B:47:GLY:HA3	1.91	0.52
1:B:126:ILE:HD12	1:B:126:ILE:N	2.24	0.52
1:A:360:LEU:C	1:A:362:ALA:H	2.17	0.52
1:B:169:ASN:O	1:B:173:VAL:HG22	2.08	0.52
1:B:262:VAL:HG12	1:B:324:LEU:HD23	1.91	0.52
1:A:4:VAL:O	1:A:219:MET:HA	2.10	0.52
1:A:25:GLU:CG	1:A:61:ARG:NH2	2.71	0.52
1:A:426:ARG:HG3	1:A:426:ARG:HH11	1.74	0.52
1:A:280:THR:HG22	1:A:309:TRP:N	2.24	0.52
1:B:406:THR:HG23	1:B:408:VAL:H	1.75	0.52
1:A:94:ARG:HG2	1:A:200:MET:CE	2.39	0.52
1:B:263:LEU:HD11	1:B:328:CYS:HB2	1.92	0.51
1:B:360:LEU:O	1:B:361:ALA:C	2.50	0.51
1:A:161:LEU:O	1:A:165:MET:HG3	2.11	0.51
1:A:301:THR:HG22	1:A:303:ARG:NH2	2.25	0.51
1:A:37:HIS:H	1:A:37:HIS:CD2	2.28	0.51
1:A:107:LEU:H	1:A:110:HIS:HD2	1.59	0.51
1:B:269:TYR:HB2	1:B:308:GLY:O	2.11	0.50
1:A:89:ARG:HD3	1:A:89:ARG:N	2.25	0.50
1:A:154:LYS:HD3	1:A:191:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PHE:O	1:A:293:GLN:HB2	2.11	0.50
1:A:396:LEU:O	1:A:400:LYS:HG3	2.11	0.50
1:B:43:LEU:CD2	1:B:47:GLY:HA3	2.37	0.50
1:B:50:THR:HG21	1:B:85:GLU:OE1	2.12	0.50
1:B:217:PHE:HB3	1:B:429:PHE:CE1	2.45	0.50
1:A:220:PHE:CD2	1:A:248:VAL:HG13	2.47	0.49
1:B:37:HIS:CD2	1:B:37:HIS:H	2.30	0.49
1:B:304:ARG:HA	1:B:304:ARG:HH11	1.75	0.49
1:A:175:TYR:HB2	1:B:170:PHE:CE2	2.48	0.49
1:B:397:ASN:HA	1:B:400:LYS:HZ2	1.78	0.48
1:A:279:PRO:HG2	1:A:311:ASP:OD2	2.12	0.48
1:A:73:VAL:CG2	1:A:133:ILE:HG12	2.42	0.48
1:A:129:THR:CG2	1:A:130:GLY:N	2.75	0.48
1:B:311:ASP:HA	1:B:344:CYS:HB3	1.94	0.48
1:B:419:ARG:HH11	1:B:419:ARG:HB2	1.77	0.48
1:A:88:ASP:C	1:A:90:GLY:H	2.22	0.48
1:A:128:THR:O	1:A:129:THR:O	2.30	0.48
1:A:426:ARG:NH1	1:A:426:ARG:CG	2.77	0.48
1:B:430:ASP:O	1:B:431:ALA:HB2	2.13	0.48
1:A:303:ARG:H	1:A:303:ARG:HE	1.62	0.48
1:B:322:ASN:O	1:B:323:SER:C	2.57	0.48
1:B:126:ILE:O	1:B:126:ILE:HG22	2.13	0.48
1:A:386:LYS:NZ	1:A:421:GLU:HG3	2.29	0.48
1:B:116:ALA:HA	1:B:119:LYS:HE3	1.95	0.48
1:A:120:ALA:O	1:A:122:GLY:N	2.46	0.47
1:A:301:THR:C	1:A:305:ARG:HH21	2.22	0.47
1:B:364:ASP:O	1:B:365:TRP:C	2.55	0.47
1:B:359:PRO:C	1:B:360:LEU:O	2.57	0.47
1:A:336:ASP:OD1	1:A:382:THR:HB	2.14	0.47
1:B:184:GLN:HE22	1:B:187:LEU:HD23	1.78	0.47
1:A:383:PHE:CE1	1:A:417:PRO:HD2	2.50	0.47
1:B:209:ASP:O	1:B:213:GLN:HG2	2.14	0.47
1:A:133:ILE:O	1:A:136:ALA:HB3	2.13	0.47
1:B:85:GLU:O	1:B:89:ARG:HG2	2.15	0.47
1:A:230:ILE:HD13	1:A:240:SER:O	2.16	0.46
1:B:6:VAL:HG22	1:B:263:LEU:HD23	1.97	0.46
1:A:172:LEU:O	1:A:177:LYS:N	2.49	0.46
1:B:83:MET:O	1:B:87:GLU:HG3	2.16	0.46
1:A:118:GLU:OE1	1:A:119:LYS:HD2	2.15	0.46
3:A:557:HOH:O	1:B:249:ALA:HB1	2.15	0.46
1:B:161:LEU:O	1:B:165:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PRO:HG2	1:A:395:ALA:CB	2.45	0.46
1:B:124:LYS:NZ	1:B:124:LYS:HB2	2.31	0.45
1:A:92:PRO:O	1:A:95:GLU:HG2	2.16	0.45
1:B:32:ARG:HD3	3:B:508:HOH:O	2.14	0.45
1:A:171:GLN:HG3	3:A:530:HOH:O	2.16	0.45
1:B:154:LYS:HD2	1:B:191:MET:SD	2.57	0.45
1:B:380:GLU:H	1:B:380:GLU:CD	2.25	0.45
1:A:115:ASN:O	1:A:116:ALA:C	2.58	0.45
1:A:347:TYR:HB3	1:A:349:MET:CE	2.46	0.45
1:A:83:MET:HE3	1:A:83:MET:HB2	1.89	0.45
1:A:385:VAL:HG12	1:A:423:MET:HE2	1.98	0.45
1:B:67:ILE:HD11	1:B:207:LEU:HD21	1.98	0.45
1:A:355:VAL:HG13	1:A:357:THR:H	1.81	0.45
1:B:14:GLU:CB	1:B:265:ILE:HG22	2.46	0.45
1:B:28:LYS:HE2	1:B:63:ASN:O	2.17	0.45
1:B:107:LEU:H	1:B:110:HIS:CD2	2.31	0.44
1:A:32:ARG:HD3	3:A:574:HOH:O	2.17	0.44
1:A:384:GLY:HA2	1:A:421:GLU:HG2	1.99	0.44
1:A:101:GLU:HA	1:A:148:VAL:HB	1.98	0.44
1:A:128:THR:HG23	3:A:486:HOH:O	2.17	0.44
1:A:173:VAL:CG2	1:A:180:ALA:HB2	2.48	0.44
1:A:301:THR:C	1:A:305:ARG:NH2	2.76	0.44
1:A:262:VAL:HG12	1:A:324:LEU:HD23	1.99	0.44
1:A:282:LEU:HD13	1:A:286:THR:HB	1.99	0.44
1:B:45:ILE:HG21	3:B:585:HOH:O	2.17	0.44
1:B:64:VAL:HG12	1:B:65:THR:N	2.31	0.44
1:A:242:ASN:ND2	1:B:250:THR:CG2	2.80	0.44
1:B:364:ASP:C	1:B:366:LYS:N	2.74	0.44
1:A:389:SER:C	1:A:391:LEU:H	2.25	0.44
1:B:303:ARG:HA	1:B:303:ARG:HD3	1.82	0.44
1:A:28:LYS:NZ	1:A:214:ARG:HH22	2.15	0.43
1:A:196:ILE:HD11	3:A:512:HOH:O	2.17	0.43
1:B:121:ARG:HG3	3:B:608:HOH:O	2.17	0.43
1:B:364:ASP:O	1:B:368:VAL:HG13	2.17	0.43
1:B:20:VAL:O	1:B:24:THR:HG23	2.18	0.43
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.79	0.43
1:B:118:GLU:HG2	1:B:127:GLY:HA3	1.99	0.43
1:A:146:LEU:HD22	1:A:157:PHE:CE1	2.54	0.43
1:A:267:LYS:HG2	1:A:330:THR:HG22	1.99	0.43
1:A:411:ASP:O	1:A:425:LEU:N	2.52	0.43
1:A:111:VAL:HG13	1:A:115:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD13	1:A:172:LEU:HD21	2.01	0.43
1:B:131:ARG:HG2	1:B:133:ILE:HD12	2.01	0.43
1:B:160:LYS:HE3	3:B:538:HOH:O	2.18	0.43
1:B:64:VAL:CG1	1:B:65:THR:N	2.82	0.42
1:B:68:ILE:HB	1:B:99:LEU:HD23	2.00	0.42
1:A:285:GLU:OE1	1:A:285:GLU:HA	2.18	0.42
1:B:24:THR:HG22	1:B:30:VAL:HG21	2.00	0.42
1:B:214:ARG:NH1	1:B:216:ASP:OD2	2.51	0.42
1:B:317:ARG:HH21	1:B:358:THR:HG22	1.85	0.42
1:A:147:ARG:O	1:A:148:VAL:C	2.61	0.42
1:A:170:PHE:CD1	1:A:170:PHE:C	2.98	0.42
1:A:412:ILE:C	1:A:413:ILE:HG13	2.44	0.42
1:A:396:LEU:HD23	1:A:399:ILE:HD12	2.02	0.42
1:B:426:ARG:HH11	1:B:426:ARG:HD3	1.69	0.42
1:A:375:MET:HA	1:A:376:PRO:HD3	1.82	0.42
1:A:4:VAL:HG22	1:A:261:TYR:HB3	2.02	0.42
1:A:165:MET:HE2	1:A:165:MET:HB3	1.57	0.42
1:B:48:GLU:HB2	1:B:49:LYS:H	1.70	0.42
1:B:418:ASP:HB3	1:B:421:GLU:HG3	2.02	0.42
1:B:319:VAL:HA	1:B:324:LEU:HD12	2.01	0.41
1:A:255:GLY:HA3	1:B:323:SER:HB3	2.02	0.41
1:B:107:LEU:N	1:B:110:HIS:HD2	2.18	0.41
1:B:348:ARG:HB2	1:B:371:ILE:HD11	2.02	0.41
1:A:261:TYR:CD1	1:A:428:PRO:HB3	2.56	0.41
1:B:419:ARG:HB2	1:B:419:ARG:NH1	2.35	0.41
1:A:358:THR:O	1:A:359:PRO:C	2.63	0.41
1:B:143:ARG:NH2	3:B:434:HOH:O	2.54	0.41
1:B:47:GLY:HA2	1:B:60:LEU:HD11	2.02	0.41
1:A:46:ASN:C	1:A:48:GLU:H	2.29	0.41
1:A:257:ARG:HD2	3:A:446:HOH:O	2.20	0.41
1:B:281:GLU:CD	1:B:306:ARG:HD2	2.46	0.41
1:A:282:LEU:HG	1:A:308:GLY:HA2	2.02	0.41
1:A:9:THR:C	1:A:10:GLN:HG3	2.46	0.41
1:A:206:ASP:OD1	1:B:320:GLN:NE2	2.53	0.41
1:A:59:ILE:CD1	1:A:96:ARG:HB2	2.51	0.41
1:A:5:VAL:HA	1:A:220:PHE:HB2	2.03	0.40
1:B:288:GLU:O	1:B:289:PHE:C	2.64	0.40
1:A:84:LYS:HA	1:A:84:LYS:HD2	1.85	0.40
1:B:128:THR:HG23	1:B:128:THR:O	2.20	0.40
1:B:411:ASP:O	1:B:425:LEU:N	2.51	0.40
1:B:427:ASP:HA	1:B:428:PRO:HD3	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:C	1:A:120:ALA:N	2.79	0.40
1:B:4:VAL:HG22	1:B:261:TYR:HB3	2.04	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:499:HOH:H1	3:B:537:HOH:O[1_565]	1.03	0.57
1:A:155:GLU:OE1	1:A:299:ALA:O[3_644]	1.72	0.48
1:A:155:GLU:OE2	1:A:299:ALA:O[3_644]	1.80	0.40
3:A:499:HOH:H1	3:B:537:HOH:H1[1_565]	1.24	0.36
1:A:155:GLU:CD	1:A:299:ALA:O[3_644]	1.86	0.34
3:A:537:HOH:O	3:A:604:HOH:H2[3_644]	1.30	0.30
3:A:499:HOH:O	3:B:537:HOH:O[1_565]	1.94	0.26
1:A:46:ASN:OD1	1:B:123:ALA:CB[3_654]	2.09	0.11
3:A:500:HOH:O	3:B:521:HOH:H2[2_565]	1.50	0.10
3:A:495:HOH:O	3:A:502:HOH:H2[3_654]	1.57	0.03
1:A:188:ASP:O	1:A:292:LYS:HZ3[3_644]	1.59	0.01
1:B:354:GLU:O	3:B:499:HOH:H1[4_555]	1.59	0.01

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	429/431 (100%)	366 (85%)	55 (13%)	8 (2%)	6	5
1	B	429/431 (100%)	391 (91%)	29 (7%)	9 (2%)	5	4
All	All	858/862 (100%)	757 (88%)	84 (10%)	17 (2%)	6	5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	362	ALA
1	B	48	GLU
1	B	361	ALA
1	A	122	GLY
1	B	299	ALA
1	A	120	ALA
1	A	297	PHE
1	A	301	THR
1	A	427	ASP
1	B	40	GLY
1	B	427	ASP
1	B	122	GLY
1	B	298	GLY
1	A	392	PRO
1	B	127	GLY
1	B	44	VAL

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%)	315 (89%)	38 (11%)	6	7
1	B	353/353 (100%)	321 (91%)	32 (9%)	9	11
All	All	706/706 (100%)	636 (90%)	70 (10%)	7	9

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	34	GLN
1	A	43	LEU
1	A	56	PRO
1	A	57	SER
1	A	62	GLU
1	A	81	LYS

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Mol	Chain	Res	Type
1	A	89	ARG
1	A	96	ARG
1	A	104	PRO
1	A	111	VAL
1	A	113	LEU
1	A	133	ILE
1	A	135	PRO
1	A	164	VAL
1	A	165	MET
1	A	207	LEU
1	A	230	ILE
1	A	266	LEU
1	A	267	LYS
1	A	292	LYS
1	A	297	PHE
1	A	300	THR
1	A	303	ARG
1	A	310	LEU
1	A	312	THR
1	A	330	THR
1	A	333	ASP
1	A	343	LEU
1	A	348	ARG
1	A	355	VAL
1	A	357	THR
1	A	369	GLU
1	A	373	GLU
1	A	382	THR
1	A	387	ASP
1	A	401	ARG
1	A	426	ARG
1	B	7	LEU
1	B	13	ASP
1	B	19	ILE
1	B	26	ARG
1	B	28	LYS
1	B	34	GLN
1	B	45	ILE
1	B	48	GLU
1	B	62	GLU
1	B	63	ASN
1	B	85	GLU

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Mol	Chain	Res	Type
1	B	124	LYS
1	B	179	GLU
1	B	193	VAL
1	B	200	MET
1	B	205	SER
1	B	207	LEU
1	B	221	GLU
1	B	239	THR
1	B	282	LEU
1	B	301	THR
1	B	310	LEU
1	B	320	GLN
1	B	330	THR
1	B	350	PRO
1	B	358	THR
1	B	364	ASP
1	B	374	THR
1	B	379	SER
1	B	382	THR
1	B	406	THR
1	B	426	ARG

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	63	ASN
1	A	110	HIS
1	A	171	GLN
1	A	210	GLN
1	A	213	GLN
1	A	397	ASN
1	B	2	ASN
1	B	37	HIS
1	B	46	ASN
1	B	53	HIS
1	B	110	HIS
1	B	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	GNH	A	432	-	29,30,30	1.39	6 (20%)	42,47,47	1.49	8 (19%)

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	GNH	A	432	-	-	3/13/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	432	GNH	PB-O2B	-3.29	1.48	1.56
2	A	432	GNH	C1'-N9	-2.82	1.39	1.47
2	A	432	GNH	PB-O3A	2.27	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	432	GNH	C2'-C3'	-2.22	1.47	1.53
2	A	432	GNH	O4'-C1'	2.05	1.46	1.42
2	A	432	GNH	C4-N9	-2.02	1.32	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	432	GNH	O4'-C1'-N9	4.11	117.66	108.36
2	A	432	GNH	O2B-PB-O3A	-2.57	96.07	104.64
2	A	432	GNH	O2A-PA-O1A	2.28	123.06	112.44
2	A	432	GNH	C8-N7-C5	-2.23	100.29	104.26
2	A	432	GNH	O3'-C3'-C2'	-2.18	104.82	111.82
2	A	432	GNH	O5'-C5'-C4'	2.14	116.28	108.99
2	A	432	GNH	N9-C8-N7	2.14	117.36	113.40
2	A	432	GNH	PB-O3A-PA	-2.02	125.63	132.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	432	GNH	C5'-O5'-PA-O3A
2	A	432	GNH	C5'-O5'-PA-O1A
2	A	432	GNH	C4'-C5'-O5'-PA

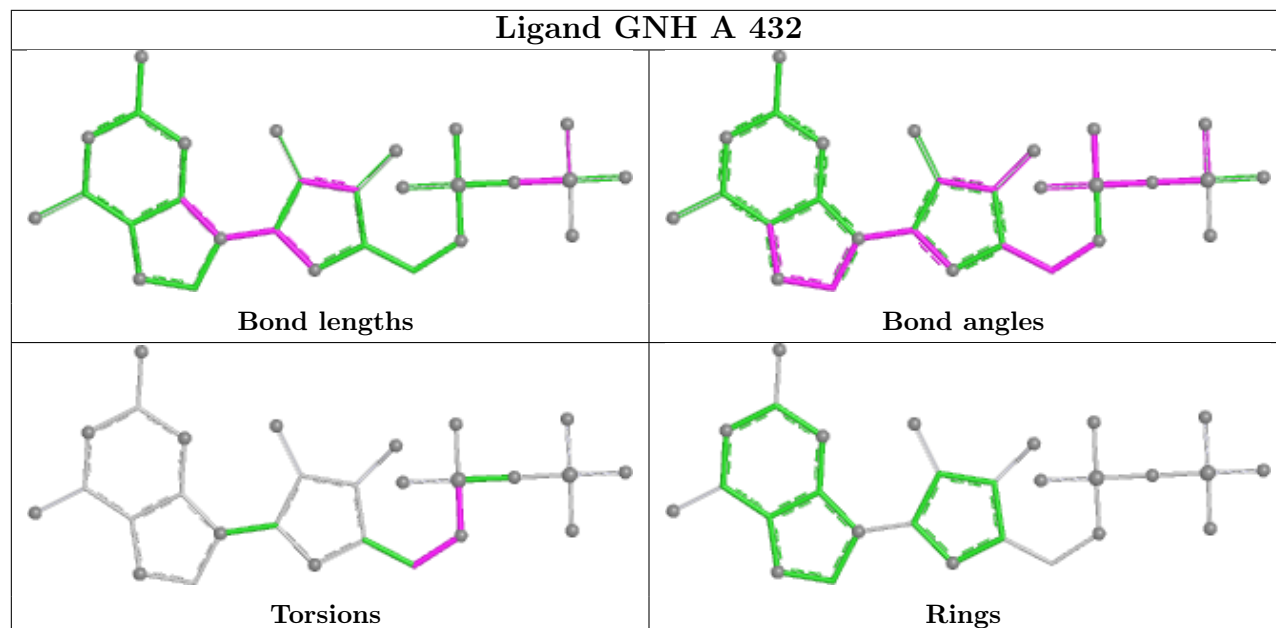
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	GNH	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](#)

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	431/431 (100%)	1.16	66 (15%) 5 6	4, 17, 40, 60	0
1	B	431/431 (100%)	0.63	31 (7%) 21 23	4, 13, 39, 60	0
All	All	862/862 (100%)	0.90	97 (11%) 10 11	4, 15, 39, 60	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	THR	5.6
1	B	362	ALA	5.0
1	A	47	GLY	4.8
1	A	127	GLY	4.6
1	B	298	GLY	4.5
1	B	44	VAL	4.4
1	A	46	ASN	4.3
1	A	299	ALA	4.3
1	B	361	ALA	4.0
1	B	122	GLY	3.9
1	B	128	THR	3.7
1	B	126	ILE	3.7
1	A	86	LEU	3.7
1	A	123	ALA	3.6
1	B	45	ILE	3.6
1	B	123	ALA	3.4
1	A	301	THR	3.4
1	A	300	THR	3.2
1	A	391	LEU	3.1
1	A	393	GLN	3.1
1	B	129	THR	3.1
1	A	125	ALA	3.1
1	A	90	GLY	3.1
1	A	418	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	390	GLY	3.0
1	A	79	LEU	3.0
1	A	400	LYS	3.0
1	B	49	LYS	2.9
1	A	420	THR	2.9
1	B	360	LEU	2.8
1	A	78	ALA	2.8
1	A	240	SER	2.8
1	A	414	SER	2.8
1	B	47	GLY	2.8
1	B	46	ASN	2.7
1	A	20	VAL	2.7
1	A	295	ASN	2.7
1	B	125	ALA	2.7
1	A	376	PRO	2.7
1	B	364	ASP	2.6
1	A	352	GLY	2.6
1	A	92	PRO	2.6
1	A	379	SER	2.6
1	A	118	GLU	2.6
1	A	180	ALA	2.6
1	A	120	ALA	2.6
1	A	135	PRO	2.6
1	A	415	THR	2.6
1	A	88	ASP	2.5
1	A	297	PHE	2.5
1	B	178	ALA	2.5
1	A	119	LYS	2.5
1	A	116	ALA	2.5
1	A	291	CYS	2.5
1	A	360	LEU	2.5
1	A	194	ALA	2.5
1	A	387	ASP	2.4
1	A	346	ALA	2.4
1	B	304	ARG	2.4
1	B	431	ALA	2.4
1	A	381	SER	2.4
1	B	374	THR	2.4
1	B	241	SER	2.4
1	A	45	ILE	2.4
1	A	17	GLY	2.3
1	A	57	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	106	ILE	2.3
1	A	302	GLY	2.3
1	A	357	THR	2.3
1	B	366	LYS	2.3
1	A	50	THR	2.3
1	A	27	ALA	2.3
1	A	280	THR	2.3
1	B	350	PRO	2.2
1	A	276	GLY	2.2
1	A	158	ALA	2.2
1	A	75	SER	2.2
1	A	63	ASN	2.2
1	A	364	ASP	2.2
1	A	149	GLY	2.2
1	A	362	ALA	2.2
1	B	300	THR	2.2
1	B	389	SER	2.2
1	A	195	ASP	2.2
1	A	58	GLY	2.2
1	B	363	ASP	2.1
1	A	184	GLN	2.1
1	A	303	ARG	2.1
1	B	303	ARG	2.1
1	B	38	ASN	2.1
1	A	181	VAL	2.1
1	A	156	THR	2.1
1	B	234	THR	2.1
1	B	299	ALA	2.1
1	A	365	TRP	2.0
1	A	286	THR	2.0
1	A	59	ILE	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](#)

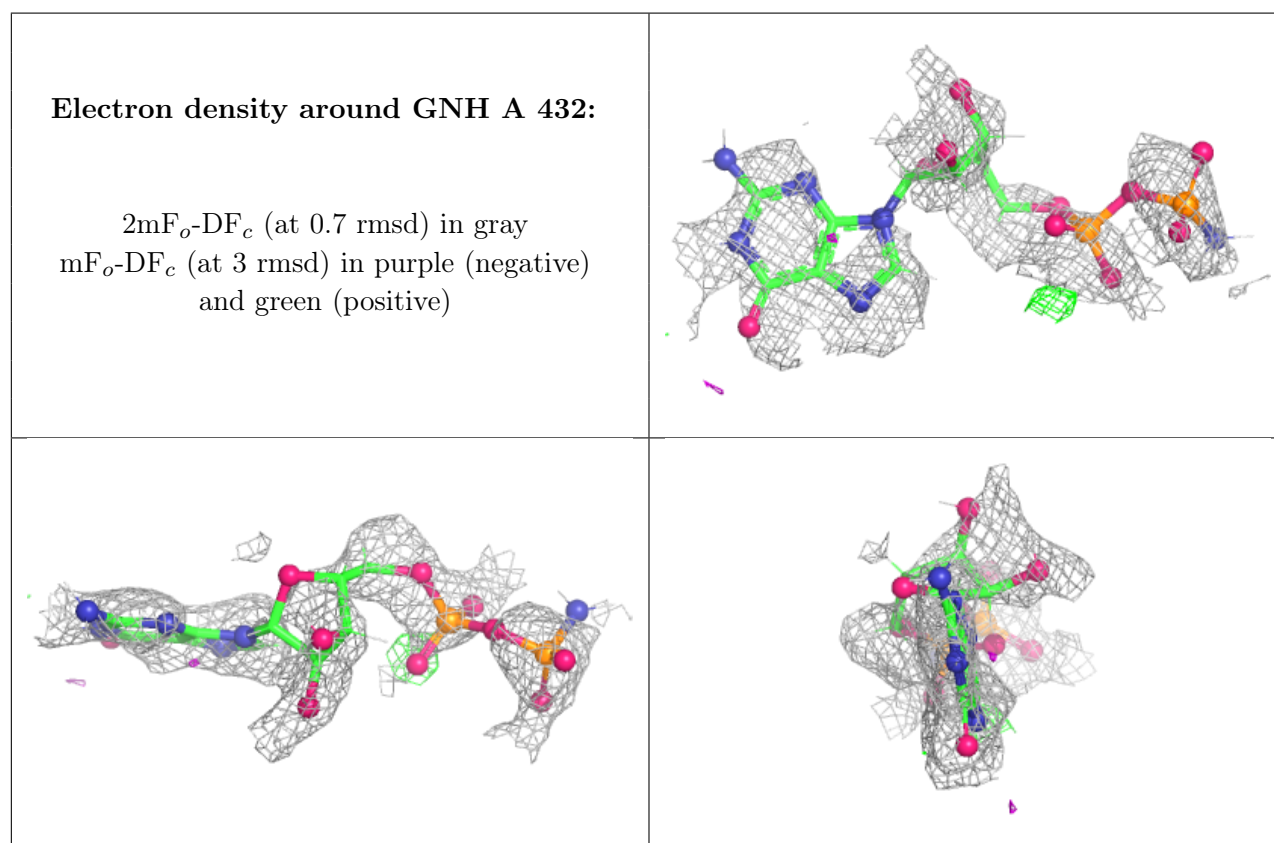
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	GNH	A	432	28/28	0.66	0.15	0,21,28,29	42

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.