



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 1HJ6 / pdb_00001hj6
Title : ISOCITRATE DEHYDROGENASE S113E MUTANT COMPLEXED WITH ISOPROPYLMALATE, NADP+ AND MAGNESIUM (FLASH-COOLED)
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Deposited on : 2001-01-08
Resolution : 2.00 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

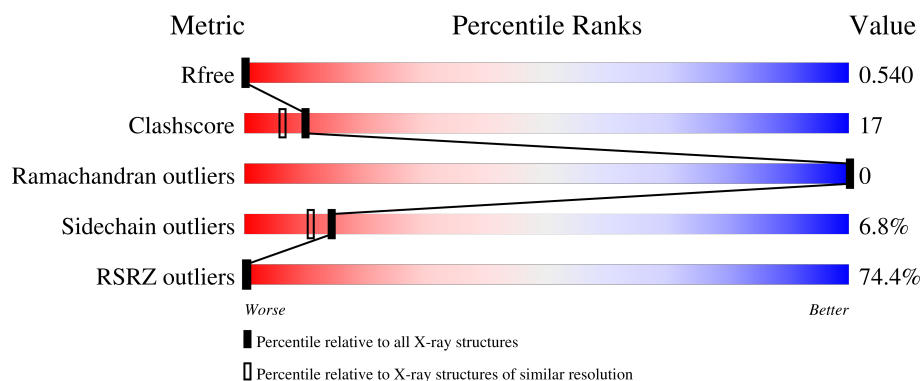
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1417	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1418	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3504 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 ISOCITRATE DEHYDROGENASE.

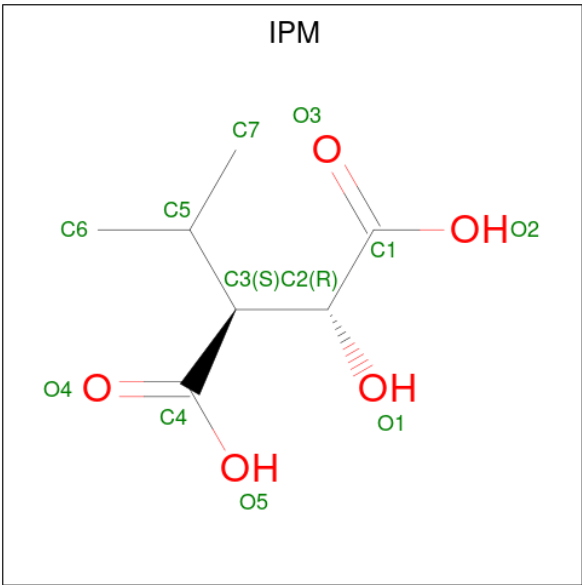
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3199	2037	538	606	18	0	0	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



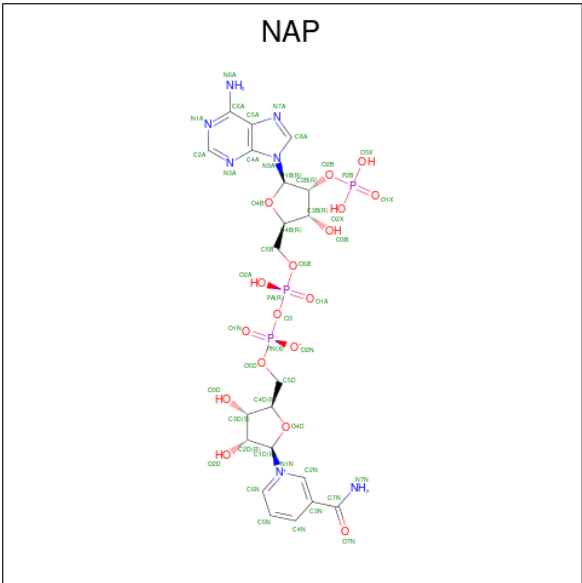
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0

- Molecule 3 is 3-ISOPROPYLMALIC ACID (CCD ID: IPM) (formula: $C_7H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	7	5		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			48	21	7	17		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

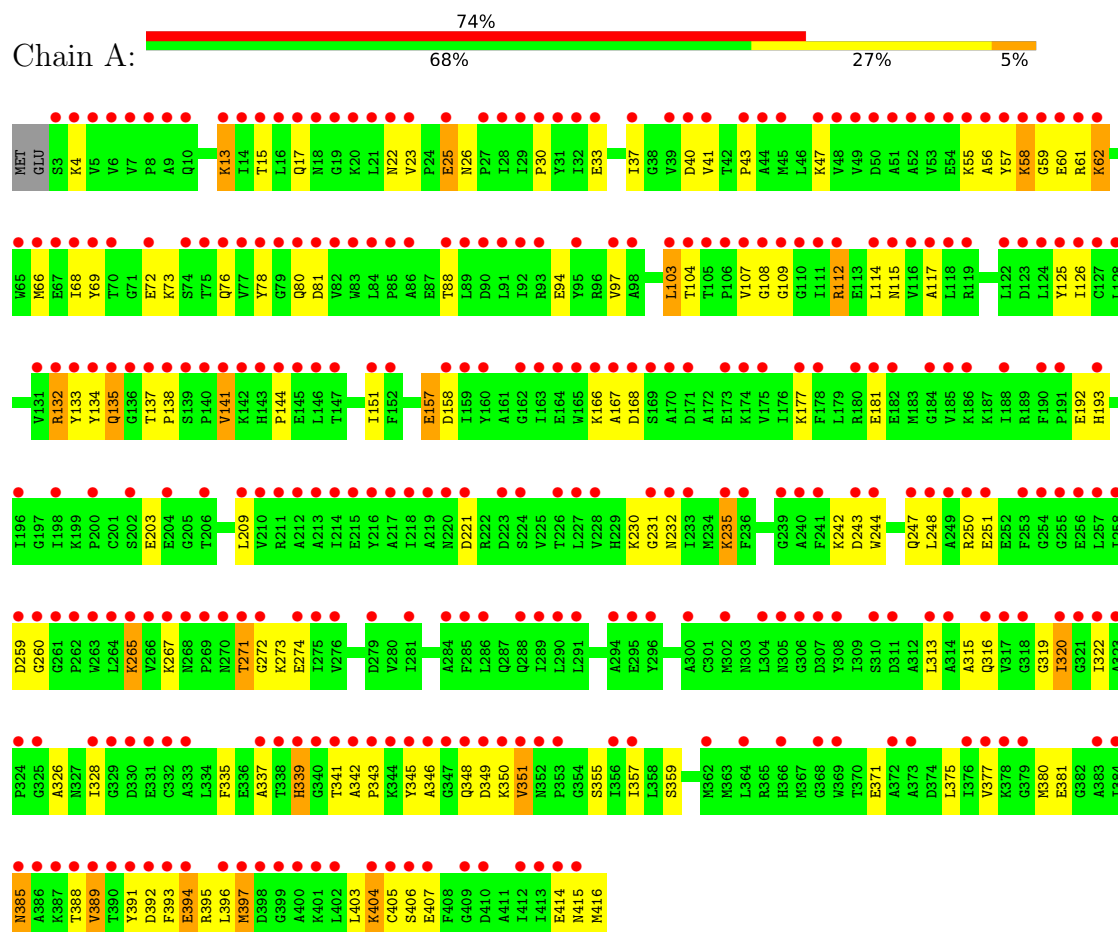
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	232	Total 232	O 232	0	0

3 Residue-property plots [i](#)

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: ISOCITRATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.30Å 102.30Å 150.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00 6.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (6.00-2.00) 94.7 (6.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.246 0.538 , 0.540	Depositor DCC
R_{free} test set	2847 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.92 , 119.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	3504	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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: IPM, MG, GOL, NAP

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	0.38	0/3260	0.87	9/4409 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	N-CA-C	7.20	115.03	107.76
1	A	69	TYR	N-CA-C	6.99	120.91	109.72
1	A	41	VAL	N-CA-C	6.71	117.50	110.72
1	A	389	VAL	N-CA-C	6.39	116.61	108.82
1	A	339	HIS	N-CA-C	5.67	117.39	110.41
1	A	235	LYS	N-CA-C	5.67	117.46	111.28
1	A	328	ILE	N-CA-C	5.66	116.09	108.17
1	A	114	LEU	N-CA-C	5.52	117.30	111.28
1	A	359	SER	N-CA-C	-5.20	105.67	112.23

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	3199	0	3223	113	50
2	A	12	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	10	0	0
4	A	48	0	25	0	0
5	A	1	0	0	0	0
6	A	232	0	0	40	1
All	All	3504	0	3266	113	51

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 17.

All (113) 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:415:ASN:N	6:A:2223:HOH:O	1.62	1.26
1:A:415:ASN:ND2	6:A:2223:HOH:O	1.63	1.24
1:A:59:GLY:CA	6:A:2033:HOH:O	1.86	1.21
1:A:416:MET:N	6:A:2224:HOH:O	1.78	1.16
1:A:109:GLY:CA	6:A:2077:HOH:O	1.93	1.15
1:A:80:GLN:CG	6:A:2056:HOH:O	2.00	1.07
1:A:232:ASN:N	6:A:2152:HOH:O	1.92	1.03
1:A:231:GLY:C	6:A:2152:HOH:O	2.01	1.03
1:A:59:GLY:N	6:A:2033:HOH:O	1.93	0.96
1:A:80:GLN:HG3	6:A:2056:HOH:O	1.61	0.96
1:A:259:ASP:CG	1:A:260:GLY:H	1.77	0.91
1:A:109:GLY:O	6:A:2077:HOH:O	1.86	0.90
1:A:416:MET:O	6:A:2224:HOH:O	1.88	0.89
1:A:415:ASN:CA	6:A:2223:HOH:O	2.10	0.84
1:A:415:ASN:CG	6:A:2223:HOH:O	1.95	0.84
1:A:80:GLN:OE1	6:A:2058:HOH:O	1.96	0.83
1:A:109:GLY:HA3	6:A:2077:HOH:O	1.69	0.79
1:A:415:ASN:CB	6:A:2223:HOH:O	2.22	0.79
1:A:80:GLN:CD	6:A:2056:HOH:O	2.27	0.76
1:A:349:ASP:OD1	1:A:405:CYS:HB3	1.85	0.76
1:A:414:GLU:C	6:A:2223:HOH:O	2.09	0.73
1:A:404:LYS:HG2	1:A:407:GLU:H	1.52	0.73
1:A:80:GLN:NE2	6:A:2058:HOH:O	2.23	0.72
1:A:59:GLY:HA3	6:A:2033:HOH:O	1.70	0.72
1:A:80:GLN:CD	6:A:2058:HOH:O	2.33	0.71
1:A:80:GLN:HB2	6:A:2056:HOH:O	1.91	0.71
1:A:389:VAL:HG21	1:A:397:MET:HE3	1.75	0.68
1:A:138:PRO:HG3	1:A:393:PHE:O	1.93	0.68
1:A:80:GLN:O	1:A:81:ASP:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLY:CA	6:A:2152:HOH:O	2.36	0.67
1:A:259:ASP:CG	1:A:260:GLY:N	2.47	0.67
1:A:416:MET:CA	6:A:2224:HOH:O	2.37	0.65
1:A:76:GLN:HG2	6:A:2053:HOH:O	1.97	0.63
1:A:112:ARG:HD2	1:A:117:ALA:HB2	1.79	0.63
1:A:13:LYS:HE2	1:A:94:GLU:HG2	1.80	0.62
1:A:166:LYS:NZ	6:A:2112:HOH:O	2.32	0.61
1:A:267:LYS:HD2	1:A:272:GLY:O	2.01	0.61
1:A:55:LYS:HG2	1:A:375:LEU:CD1	2.31	0.61
1:A:43:PRO:O	1:A:47:LYS:HG3	2.01	0.60
1:A:192:GLU:HB3	1:A:193:HIS:CD2	2.37	0.59
1:A:337:ALA:HB1	1:A:355:SER:HB3	1.85	0.59
1:A:138:PRO:HB3	1:A:397:MET:HG2	1.85	0.58
1:A:138:PRO:HG3	1:A:397:MET:HG3	1.86	0.58
1:A:377:VAL:O	1:A:381:GLU:HG3	2.04	0.58
1:A:265:LYS:HG2	1:A:265:LYS:O	2.03	0.57
1:A:341:THR:O	1:A:342:ALA:C	2.48	0.57
1:A:13:LYS:HE2	1:A:94:GLU:CG	2.35	0.57
1:A:416:MET:C	6:A:2224:HOH:O	2.41	0.56
1:A:404:LYS:HG2	1:A:407:GLU:HB2	1.88	0.55
1:A:404:LYS:CE	1:A:407:GLU:HG3	2.37	0.55
1:A:395:ARG:HD3	6:A:2218:HOH:O	2.07	0.54
1:A:151:ILE:HD11	1:A:313:LEU:HD12	1.88	0.54
1:A:80:GLN:CB	6:A:2056:HOH:O	2.35	0.53
1:A:55:LYS:HG2	1:A:375:LEU:HD11	1.89	0.53
1:A:177:LYS:O	1:A:181:GLU:HB2	2.09	0.53
1:A:391:TYR:CG	1:A:392:ASP:N	2.78	0.52
1:A:313:LEU:O	1:A:316:GLN:HB2	2.10	0.52
1:A:388:THR:HB	1:A:403:LEU:HD11	1.92	0.52
1:A:404:LYS:HE2	1:A:407:GLU:HG3	1.92	0.52
1:A:177:LYS:HZ2	1:A:181:GLU:CD	2.19	0.51
1:A:132:ARG:HD2	1:A:134:TYR:CE1	2.46	0.51
1:A:230:LYS:HE3	1:A:232:ASN:OD1	2.11	0.51
1:A:393:PHE:O	1:A:397:MET:HG3	2.12	0.50
1:A:133:TYR:CD1	1:A:144:PRO:HB2	2.47	0.50
1:A:267:LYS:HD3	1:A:274:GLU:OE2	2.12	0.50
1:A:251:GLU:HG2	6:A:2162:HOH:O	2.11	0.49
1:A:345:TYR:O	1:A:348:GLN:HB2	2.12	0.49
1:A:158:ASP:HB2	6:A:2098:HOH:O	2.14	0.48
1:A:30:PRO:HA	1:A:66:MET:O	2.13	0.48
1:A:73:LYS:HA	1:A:76:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:O	1:A:396:LEU:HD23	2.14	0.47
1:A:40:ASP:O	1:A:43:PRO:HD2	2.14	0.47
1:A:221:ASP:CG	1:A:271:THR:HG21	2.38	0.47
1:A:192:GLU:HB2	6:A:2132:HOH:O	2.14	0.47
1:A:26:ASN:HA	1:A:62:LYS:O	2.15	0.47
1:A:141:VAL:HG11	1:A:316:GLN:HG2	1.98	0.47
1:A:157:GLU:HB2	1:A:158:ASP:H	1.47	0.46
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.96	0.46
1:A:33:GLU:HG2	6:A:2015:HOH:O	2.16	0.46
1:A:58:LYS:C	6:A:2033:HOH:O	2.48	0.46
1:A:135:GLN:CD	1:A:385:ASN:HD21	2.24	0.46
1:A:343:PRO:HA	1:A:346:ALA:HB2	1.98	0.45
1:A:17:GLN:HE22	1:A:22:ASN:HD22	1.63	0.45
1:A:133:TYR:CE1	1:A:137:THR:HB	2.52	0.45
1:A:30:PRO:HD2	1:A:97:VAL:O	2.17	0.44
1:A:273:LYS:HD2	6:A:2147:HOH:O	2.17	0.44
1:A:80:GLN:NE2	6:A:2056:HOH:O	2.45	0.43
1:A:231:GLY:HA3	6:A:2152:HOH:O	2.14	0.43
1:A:404:LYS:HE3	1:A:407:GLU:HG3	2.00	0.43
1:A:15:THR:OG1	1:A:22:ASN:HB3	2.18	0.43
1:A:247:GLN:NE2	6:A:2158:HOH:O	2.48	0.43
1:A:389:VAL:CG2	1:A:397:MET:HE3	2.45	0.43
1:A:403:LEU:HD22	1:A:407:GLU:HB3	2.00	0.43
1:A:320:ILE:HD13	1:A:339:HIS:HA	2.01	0.42
1:A:357:ILE:HG21	1:A:380:MET:HE1	2.01	0.42
1:A:17:GLN:NE2	1:A:22:ASN:HD22	2.17	0.42
1:A:326:ALA:HB2	1:A:335:PHE:CD2	2.54	0.42
1:A:209:LEU:C	1:A:209:LEU:HD13	2.44	0.42
1:A:394:GLU:O	1:A:397:MET:HB2	2.19	0.42
1:A:395:ARG:O	1:A:396:LEU:HB3	2.20	0.42
1:A:380:MET:HE2	1:A:380:MET:HB2	1.83	0.42
1:A:315:ALA:HA	1:A:319:GLY:HA2	2.02	0.42
1:A:68:ILE:HD12	1:A:88:THR:HG23	2.02	0.41
1:A:103:LEU:HB2	1:A:115:ASN:HD21	1.84	0.41
1:A:4:LYS:HG3	1:A:78:TYR:CE2	2.55	0.41
1:A:167:ALA:O	1:A:168:ASP:HB2	2.20	0.41
1:A:388:THR:HB	1:A:403:LEU:CD1	2.50	0.41
1:A:59:GLY:HA2	6:A:2033:HOH:O	1.81	0.41
1:A:322:ILE:O	1:A:322:ILE:HG23	2.21	0.41
1:A:203:GLU:HG3	1:A:244:TRP:CD1	2.56	0.41
1:A:125:TYR:CD1	1:A:126:ILE:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:CD2	1:A:61:ARG:HD2	2.55	0.40
1:A:395:ARG:O	1:A:396:LEU:CB	2.69	0.40

All (51) 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)
1:A:109:GLY:N	1:A:371:GLU:OE2[4_535]	0.62	1.58
1:A:250:ARG:NH2	1:A:414:GLU:C[5_354]	0.75	1.45
1:A:56:ALA:C	1:A:107:VAL:CB[3_344]	0.80	1.40
1:A:109:GLY:CA	1:A:371:GLU:OE2[4_535]	0.95	1.25
1:A:109:GLY:N	1:A:371:GLU:CD[4_535]	0.97	1.23
1:A:56:ALA:O	1:A:107:VAL:CB[3_344]	0.98	1.22
1:A:250:ARG:NH2	1:A:414:GLU:CA[5_354]	1.14	1.06
1:A:250:ARG:CZ	1:A:414:GLU:CA[5_354]	1.14	1.06
1:A:57:TYR:N	1:A:107:VAL:CG2[3_344]	1.18	1.02
1:A:56:ALA:C	1:A:107:VAL:CG2[3_344]	1.28	0.92
1:A:56:ALA:CA	1:A:107:VAL:CG1[3_344]	1.32	0.88
1:A:56:ALA:C	1:A:107:VAL:CG1[3_344]	1.35	0.85
1:A:250:ARG:NE	1:A:414:GLU:CA[5_354]	1.42	0.78
1:A:250:ARG:NH2	1:A:414:GLU:O[5_354]	1.43	0.77
1:A:56:ALA:O	1:A:107:VAL:CG1[3_344]	1.44	0.76
1:A:56:ALA:O	1:A:107:VAL:CA[3_344]	1.50	0.70
1:A:60:GLU:OE1	1:A:104:THR:CG2[3_344]	1.53	0.67
1:A:250:ARG:NE	1:A:414:GLU:CG[5_354]	1.56	0.64
1:A:57:TYR:N	1:A:107:VAL:CB[3_344]	1.58	0.62
1:A:57:TYR:CA	1:A:107:VAL:CG2[3_344]	1.59	0.61
1:A:250:ARG:NE	1:A:414:GLU:CB[5_354]	1.60	0.60
1:A:56:ALA:O	1:A:107:VAL:CG2[3_344]	1.61	0.59
1:A:57:TYR:CE1	1:A:107:VAL:O[3_344]	1.61	0.59
1:A:250:ARG:CB	1:A:414:GLU:CG[5_354]	1.70	0.50
1:A:108:GLY:CA	1:A:371:GLU:CG[4_535]	1.72	0.48
1:A:250:ARG:CD	1:A:414:GLU:CG[5_354]	1.85	0.35
1:A:108:GLY:C	1:A:371:GLU:CD[4_535]	1.87	0.33
1:A:108:GLY:C	1:A:371:GLU:OE2[4_535]	1.87	0.33
1:A:25:GLU:OE1	1:A:72:GLU:OE1[3_344]	1.88	0.32
1:A:109:GLY:N	1:A:371:GLU:CG[4_535]	1.90	0.30
1:A:250:ARG:CB	1:A:414:GLU:CD[5_354]	1.91	0.29
1:A:250:ARG:NH2	1:A:415:ASN:N[5_354]	1.94	0.26
1:A:109:GLY:CA	1:A:371:GLU:CD[4_535]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:OE2	1:A:104:THR:OG1[3_344]	2.02	0.18
1:A:109:GLY:C	1:A:371:GLU:OE2[4_535]	2.02	0.18
1:A:250:ARG:CZ	1:A:414:GLU:C[5_354]	2.04	0.16
1:A:55:LYS:NZ	1:A:243:ASP:OD2[5_344]	2.07	0.13
1:A:57:TYR:CD1	1:A:107:VAL:N[3_344]	2.07	0.13
1:A:109:GLY:N	1:A:371:GLU:OE1[4_535]	2.07	0.13
1:A:60:GLU:CD	1:A:104:THR:CG2[3_344]	2.09	0.11
1:A:56:ALA:CA	1:A:107:VAL:CB[3_344]	2.11	0.09
1:A:60:GLU:CD	1:A:104:THR:OG1[3_344]	2.11	0.09
1:A:108:GLY:C	1:A:371:GLU:CG[4_535]	2.11	0.09
1:A:250:ARG:CG	1:A:414:GLU:CG[5_354]	2.11	0.09
1:A:250:ARG:CZ	1:A:414:GLU:N[5_354]	2.12	0.08
6:A:2032:HOH:O	6:A:2152:HOH:O[5_344]	2.15	0.05
1:A:25:GLU:CD	1:A:72:GLU:OE1[3_344]	2.16	0.04
1:A:55:LYS:CE	1:A:243:ASP:OD1[5_344]	2.16	0.04
1:A:56:ALA:CB	1:A:107:VAL:CG1[3_344]	2.16	0.04
1:A:57:TYR:CD1	1:A:107:VAL:O[3_344]	2.17	0.03
1:A:250:ARG:NE	1:A:414:GLU:N[5_354]	2.17	0.03

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	412/416 (99%)	388 (94%)	24 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	336/338 (99%)	313 (93%)	23 (7%)	14	11

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	25	GLU
1	A	58	LYS
1	A	62	LYS
1	A	103	LEU
1	A	112	ARG
1	A	132	ARG
1	A	135	GLN
1	A	141	VAL
1	A	157	GLU
1	A	235	LYS
1	A	242	LYS
1	A	248	LEU
1	A	265	LYS
1	A	271	THR
1	A	320	ILE
1	A	350	LYS
1	A	351	VAL
1	A	385	ASN
1	A	394	GLU
1	A	397	MET
1	A	404	LYS
1	A	406	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	GLN
1	A	115	ASN
1	A	135	GLN
1	A	193	HIS
1	A	270	ASN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	385	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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	IPM	A	1419	5	11,11,11	2.38	2 (18%)	11,15,15	1.36	3 (27%)
4	NAP	A	1420	-	50,52,52	1.83	11 (22%)	71,80,80	1.69	14 (19%)
2	GOL	A	1417	-	5,5,5	4.58	4 (80%)	5,5,5	6.15	3 (60%)
2	GOL	A	1418	-	5,5,5	4.59	4 (80%)	5,5,5	6.14	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPM	A	1419	5	-	4/16/16/16	-
4	NAP	A	1420	-	-	5/35/67/67	0/5/5/5
2	GOL	A	1417	-	-	2/4/4/4	-
2	GOL	A	1418	-	-	2/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1418	GOL	C3-C2	-7.99	1.21	1.51
2	A	1417	GOL	C3-C2	-7.95	1.21	1.51
4	A	1420	NAP	C2N-N1N	7.28	1.43	1.35
3	A	1419	IPM	O4-C4	4.93	1.36	1.22
3	A	1419	IPM	O3-C1	4.76	1.36	1.22
2	A	1418	GOL	O1-C1	4.65	1.61	1.42
2	A	1417	GOL	O1-C1	4.60	1.61	1.42
4	A	1420	NAP	C3N-C7N	-4.44	1.44	1.50
2	A	1417	GOL	O3-C3	3.51	1.57	1.42
4	A	1420	NAP	C6N-N1N	3.45	1.43	1.35
2	A	1418	GOL	O3-C3	3.41	1.56	1.42
4	A	1420	NAP	C4A-N3A	3.15	1.40	1.34
4	A	1420	NAP	C2A-N3A	2.89	1.39	1.33
2	A	1417	GOL	O2-C2	-2.85	1.35	1.43
4	A	1420	NAP	C5N-C4N	2.76	1.43	1.38
2	A	1418	GOL	O2-C2	-2.76	1.35	1.43
4	A	1420	NAP	C4N-C3N	2.61	1.43	1.39
4	A	1420	NAP	P2B-O2B	2.59	1.64	1.59
4	A	1420	NAP	C2N-C3N	2.22	1.42	1.39
4	A	1420	NAP	PN-O3	2.18	1.61	1.59
4	A	1420	NAP	C5A-C6A	2.01	1.46	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1417	GOL	O3-C3-C2	11.20	160.79	110.38
2	A	1418	GOL	O3-C3-C2	11.18	160.71	110.38
2	A	1417	GOL	O2-C2-C3	7.19	138.94	109.18
2	A	1418	GOL	O2-C2-C3	7.15	138.79	109.18
4	A	1420	NAP	O4B-C1B-N9A	7.13	121.79	108.09
4	A	1420	NAP	N3A-C2A-N1A	-4.46	121.83	128.58
4	A	1420	NAP	C3B-C2B-C1B	-3.94	95.26	102.81
2	A	1418	GOL	O1-C1-C2	3.44	125.88	110.38
2	A	1417	GOL	O1-C1-C2	3.44	125.86	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1420	NAP	C4D-O4D-C1D	2.96	112.63	109.92
4	A	1420	NAP	C3N-C7N-N7N	2.87	121.27	117.74
4	A	1420	NAP	O5B-C5B-C4B	2.54	117.66	108.99
4	A	1420	NAP	O4B-C1B-C2B	-2.52	102.25	106.59
4	A	1420	NAP	O2N-PN-O1N	2.51	124.13	112.44
4	A	1420	NAP	C2A-N1A-C6A	2.50	122.84	118.73
4	A	1420	NAP	O4B-C4B-C3B	-2.33	100.52	105.15
4	A	1420	NAP	O3B-C3B-C4B	2.29	117.66	111.08
3	A	1419	IPM	O2-C1-C2	2.27	119.63	113.31
4	A	1420	NAP	O7N-C7N-N7N	-2.23	119.40	122.62
4	A	1420	NAP	PN-O5D-C5D	2.16	133.73	121.35
4	A	1420	NAP	O3B-C3B-C2B	2.09	117.02	111.19
3	A	1419	IPM	O5-C4-O4	-2.06	119.41	124.08
3	A	1419	IPM	O2-C1-O3	-2.01	119.52	124.08

There are no chirality outliers.

All (13) torsion outliers are listed below:

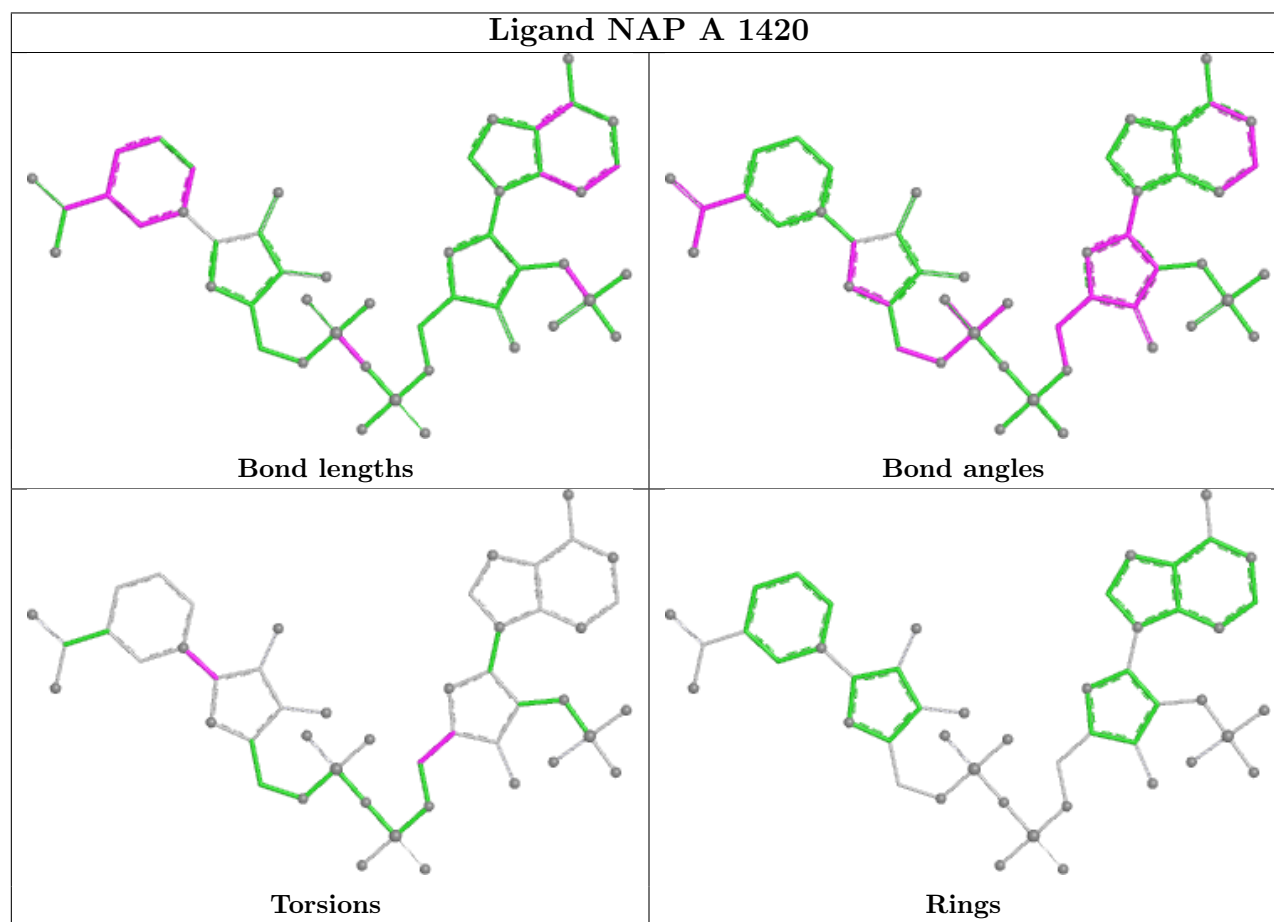
Mol	Chain	Res	Type	Atoms
2	A	1417	GOL	O1-C1-C2-C3
2	A	1417	GOL	C1-C2-C3-O3
2	A	1418	GOL	O1-C1-C2-C3
2	A	1418	GOL	C1-C2-C3-O3
4	A	1420	NAP	O4D-C1D-N1N-C2N
4	A	1420	NAP	O4D-C1D-N1N-C6N
4	A	1420	NAP	C3B-C4B-C5B-O5B
4	A	1420	NAP	O4B-C4B-C5B-O5B
3	A	1419	IPM	C1-C2-C3-C4
3	A	1419	IPM	C5-C3-C4-O5
3	A	1419	IPM	C2-C3-C4-O4
3	A	1419	IPM	C2-C3-C4-O5
4	A	1420	NAP	C2D-C1D-N1N-C2N

There are no ring outliers.

No monomer is involved in short contacts.

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	414/416 (99%)	3.05	308 (74%) 0 0	20, 31, 57, 90	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	GLY	11.6
1	A	399	GLY	9.0
1	A	398	ASP	8.9
1	A	405	CYS	7.7
1	A	404	LYS	7.0
1	A	259	ASP	6.8
1	A	168	ASP	6.7
1	A	78	TYR	6.7
1	A	9	ALA	6.6
1	A	8	PRO	6.5
1	A	139	SER	6.4
1	A	16	LEU	6.2
1	A	254	GLY	6.2
1	A	106	PRO	6.1
1	A	18	ASN	6.0
1	A	271	THR	6.0
1	A	138	PRO	6.0
1	A	212	ALA	5.9
1	A	124	LEU	5.9
1	A	333	ALA	5.8
1	A	56	ALA	5.7
1	A	219	ALA	5.7
1	A	107	VAL	5.5
1	A	110	GLY	5.5
1	A	169	SER	5.4
1	A	141	VAL	5.3
1	A	20	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	396	LEU	5.2
1	A	4	LYS	5.2
1	A	217	ALA	5.1
1	A	223	ASP	5.1
1	A	400	ALA	5.1
1	A	136	GLY	5.1
1	A	190	PHE	5.0
1	A	17	GLN	5.0
1	A	57	TYR	5.0
1	A	321	GLY	5.0
1	A	393	PHE	5.0
1	A	345	TYR	5.0
1	A	86	ALA	4.9
1	A	221	ASP	4.9
1	A	10	GLN	4.9
1	A	261	GLY	4.9
1	A	258	ILE	4.9
1	A	145	GLU	4.9
1	A	316	GLN	4.9
1	A	348	GLN	4.9
1	A	397	MET	4.9
1	A	332	CYS	4.9
1	A	391	TYR	4.9
1	A	43	PRO	4.8
1	A	144	PRO	4.8
1	A	82	VAL	4.8
1	A	137	THR	4.8
1	A	191	PRO	4.7
1	A	133	TYR	4.7
1	A	170	ALA	4.7
1	A	257	LEU	4.7
1	A	386	ALA	4.6
1	A	270	ASN	4.6
1	A	387	LYS	4.6
1	A	264	LEU	4.6
1	A	186	LYS	4.6
1	A	388	THR	4.5
1	A	19	GLY	4.5
1	A	284	ALA	4.5
1	A	322	ILE	4.4
1	A	84	LEU	4.4
1	A	134	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	181	GLU	4.4
1	A	340	GLY	4.4
1	A	143	HIS	4.4
1	A	389	VAL	4.4
1	A	182	GLU	4.4
1	A	317	VAL	4.3
1	A	351	VAL	4.3
1	A	401	LYS	4.3
1	A	385	ASN	4.3
1	A	27	PRO	4.3
1	A	295	GLU	4.3
1	A	311	ASP	4.2
1	A	30	PRO	4.2
1	A	410	ASP	4.2
1	A	251	GLU	4.2
1	A	51	ALA	4.2
1	A	346	ALA	4.2
1	A	274	GLU	4.2
1	A	185	VAL	4.2
1	A	343	PRO	4.1
1	A	50	ASP	4.1
1	A	377	VAL	4.1
1	A	85	PRO	4.1
1	A	239	GLY	4.1
1	A	269	PRO	4.1
1	A	356	ILE	4.1
1	A	83	TRP	4.0
1	A	233	ILE	4.0
1	A	243	ASP	4.0
1	A	49	VAL	4.0
1	A	228	VAL	4.0
1	A	415	ASN	4.0
1	A	392	ASP	4.0
1	A	122	LEU	3.9
1	A	344	LYS	3.9
1	A	342	ALA	3.9
1	A	268	ASN	3.9
1	A	25	GLU	3.9
1	A	6	VAL	3.9
1	A	39	VAL	3.9
1	A	40	ASP	3.9
1	A	68	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	3.9
1	A	77	VAL	3.8
1	A	231	GLY	3.8
1	A	171	ASP	3.8
1	A	330	ASP	3.8
1	A	79	GLY	3.8
1	A	127	CYS	3.8
1	A	81	ASP	3.8
1	A	265	LYS	3.8
1	A	31	TYR	3.7
1	A	414	GLU	3.7
1	A	76	GLN	3.7
1	A	409	GLY	3.6
1	A	55	LYS	3.6
1	A	104	THR	3.6
1	A	215	GLU	3.6
1	A	177	LYS	3.6
1	A	5	VAL	3.6
1	A	52	ALA	3.6
1	A	23	VAL	3.6
1	A	48	VAL	3.6
1	A	116	VAL	3.6
1	A	213	ALA	3.6
1	A	407	GLU	3.6
1	A	296	TYR	3.6
1	A	3	SER	3.6
1	A	47	LYS	3.5
1	A	290	LEU	3.5
1	A	224	SER	3.5
1	A	95	TYR	3.5
1	A	90	ASP	3.5
1	A	140	PRO	3.5
1	A	353	PRO	3.5
1	A	338	THR	3.5
1	A	275	ILE	3.5
1	A	413	ILE	3.5
1	A	162	GLY	3.4
1	A	306	GLY	3.4
1	A	105	THR	3.4
1	A	272	GLY	3.4
1	A	300	ALA	3.4
1	A	93	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	72	GLU	3.3
1	A	142	LYS	3.3
1	A	159	ILE	3.3
1	A	412	ILE	3.3
1	A	147	THR	3.3
1	A	59	GLY	3.3
1	A	69	TYR	3.3
1	A	131	VAL	3.3
1	A	175	VAL	3.3
1	A	372	ALA	3.3
1	A	54	GLU	3.3
1	A	240	ALA	3.2
1	A	253	PHE	3.2
1	A	135	GLN	3.2
1	A	260	GLY	3.2
1	A	369	TRP	3.2
1	A	331	GLU	3.2
1	A	394	GLU	3.2
1	A	373	ALA	3.2
1	A	357	ILE	3.2
1	A	41	VAL	3.2
1	A	128	LEU	3.2
1	A	255	GLY	3.2
1	A	98	ALA	3.1
1	A	379	GLY	3.1
1	A	53	VAL	3.1
1	A	67	GLU	3.1
1	A	266	VAL	3.1
1	A	368	GLY	3.1
1	A	289	ILE	3.1
1	A	347	GLY	3.0
1	A	22	ASN	3.0
1	A	58	LYS	3.0
1	A	29	ILE	3.0
1	A	232	ASN	3.0
1	A	263	TRP	3.0
1	A	123	ASP	3.0
1	A	288	GLN	3.0
1	A	218	ILE	3.0
1	A	324	PRO	3.0
1	A	339	HIS	3.0
1	A	402	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	248	LEU	2.9
1	A	28	ILE	2.9
1	A	70	THR	2.9
1	A	262	PRO	2.9
1	A	337	ALA	2.9
1	A	250	ARG	2.9
1	A	352	ASN	2.9
1	A	286	LEU	2.9
1	A	304	LEU	2.9
1	A	193	HIS	2.9
1	A	132	ARG	2.9
1	A	184	GLY	2.9
1	A	227	LEU	2.8
1	A	328	ILE	2.8
1	A	376	ILE	2.8
1	A	383	ALA	2.8
1	A	32	ILE	2.8
1	A	111	ILE	2.8
1	A	198	ILE	2.8
1	A	89	LEU	2.8
1	A	406	SER	2.8
1	A	390	THR	2.8
1	A	276	VAL	2.8
1	A	92	ILE	2.8
1	A	152	PHE	2.7
1	A	180	ARG	2.7
1	A	7	VAL	2.7
1	A	307	ASP	2.7
1	A	13	LYS	2.7
1	A	285	PHE	2.7
1	A	206	THR	2.7
1	A	188	ILE	2.7
1	A	384	ILE	2.7
1	A	310	SER	2.7
1	A	244	TRP	2.7
1	A	37	ILE	2.7
1	A	173	GLU	2.6
1	A	114	LEU	2.6
1	A	33	GLU	2.6
1	A	323	ALA	2.6
1	A	174	LYS	2.6
1	A	44	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	178	PHE	2.6
1	A	166	LYS	2.6
1	A	158	ASP	2.6
1	A	256	GLU	2.5
1	A	214	ILE	2.5
1	A	118	LEU	2.5
1	A	364	LEU	2.5
1	A	241	PHE	2.5
1	A	281	ILE	2.5
1	A	305	ASN	2.5
1	A	329	GLY	2.5
1	A	210	VAL	2.5
1	A	349	ASP	2.5
1	A	204	GLU	2.5
1	A	109	GLY	2.5
1	A	320	ILE	2.5
1	A	66	MET	2.4
1	A	165	TRP	2.4
1	A	302	MET	2.4
1	A	61	ARG	2.4
1	A	378	LYS	2.4
1	A	146	LEU	2.4
1	A	366	HIS	2.4
1	A	14	ILE	2.4
1	A	163	ILE	2.4
1	A	112	ARG	2.4
1	A	117	ALA	2.4
1	A	294	ALA	2.4
1	A	21	LEU	2.4
1	A	74	SER	2.4
1	A	15	THR	2.3
1	A	314	ALA	2.3
1	A	151	ILE	2.3
1	A	226	THR	2.3
1	A	119	ARG	2.3
1	A	211	ARG	2.3
1	A	167	ALA	2.3
1	A	249	ALA	2.3
1	A	313	LEU	2.3
1	A	362	MET	2.3
1	A	65	TRP	2.3
1	A	80	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	2.2
1	A	341	THR	2.2
1	A	220	ASN	2.2
1	A	235	LYS	2.2
1	A	45	MET	2.2
1	A	125	TYR	2.2
1	A	126	ILE	2.2
1	A	160	TYR	2.2
1	A	308	TYR	2.2
1	A	88	THR	2.2
1	A	97	VAL	2.2
1	A	291	LEU	2.2
1	A	164	GLU	2.1
1	A	236	PHE	2.1
1	A	202	SER	2.1
1	A	216	TYR	2.1
1	A	279	ASP	2.1
1	A	325	GLY	2.1
1	A	91	LEU	2.1
1	A	209	LEU	2.1
1	A	247	GLN	2.1
1	A	318	GLY	2.1
1	A	62	LYS	2.1
1	A	350	LYS	2.0
1	A	60	GLU	2.0
1	A	115	ASN	2.0
1	A	103	LEU	2.0
1	A	267	LYS	2.0
1	A	75	THR	2.0

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

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

6.3 Carbohydrates ⓘ

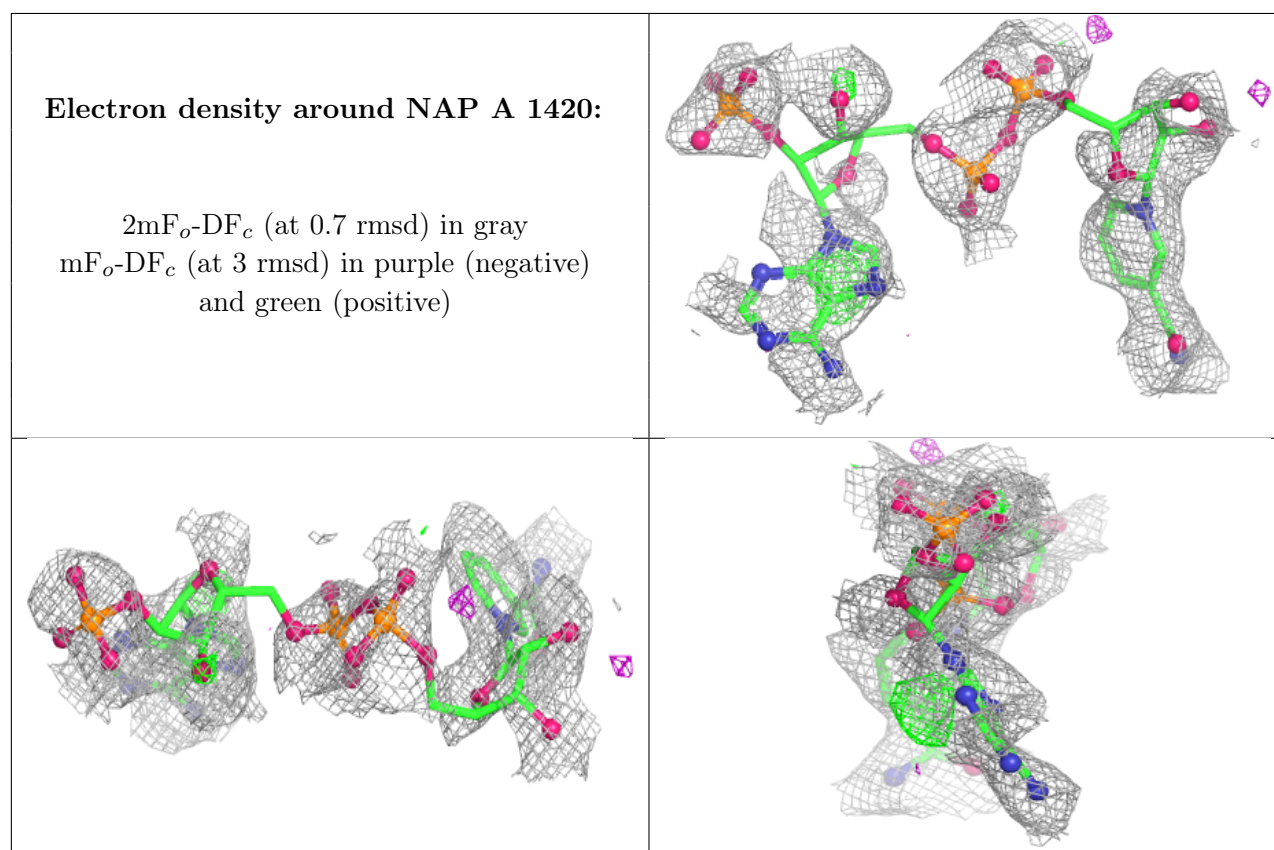
There are no oligosaccharides in this entry.

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	GOL	A	1418	6/6	0.02	0.25	64,71,73,75	0
2	GOL	A	1417	6/6	0.34	0.27	67,83,85,87	0
3	IPM	A	1419	12/12	0.55	0.24	25,29,34,37	0
5	MG	A	1421	1/1	0.59	0.16	26,26,26,26	0
4	NAP	A	1420	48/48	0.67	0.21	28,47,53,56	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.