Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 03:47 pm BST

PDB ID	:	1HJ6
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 (i) 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 (i)) were used in the production of this report:

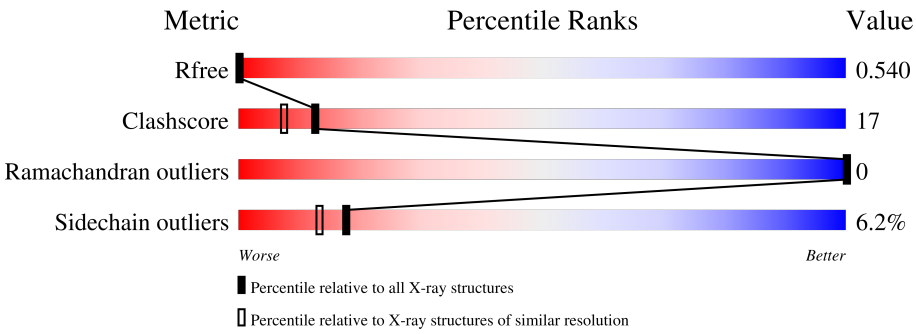
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	416	70% 25% •

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	-	-
2	GOL	A	1418	-	X	-	-

2 Entry composition (i)

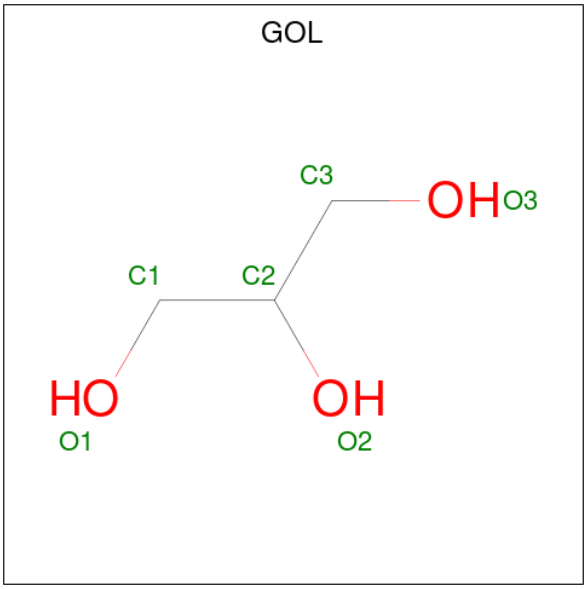
There are 6 unique types of molecules in this entry. The entry contains 3504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

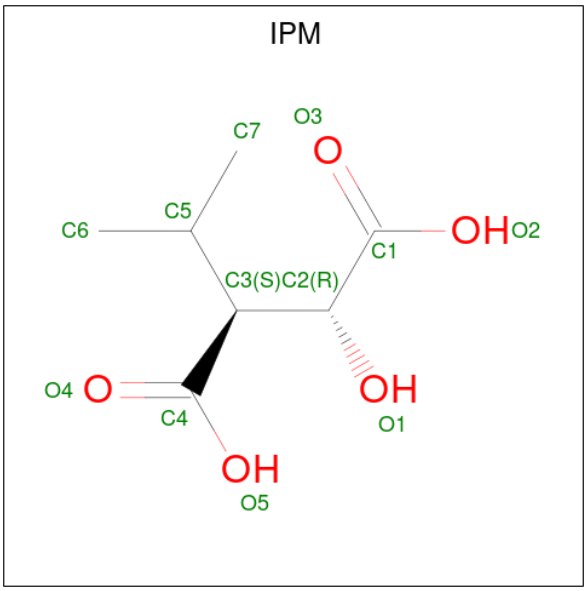
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3199	2037	538	606	18	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



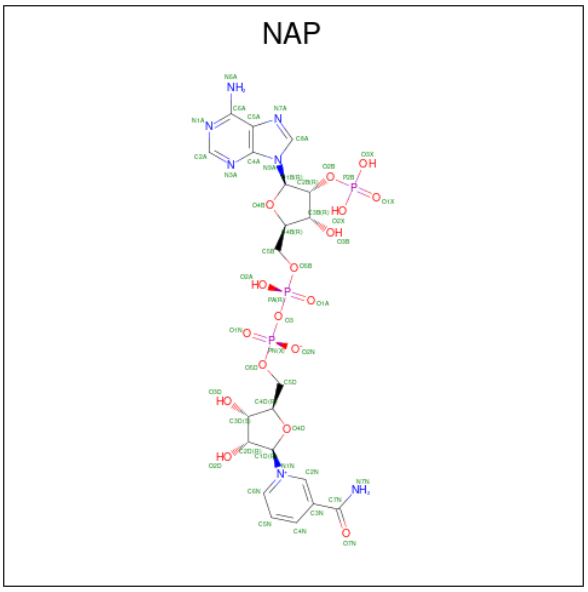
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is 3-ISOPROPYLMALIC ACID (three-letter code: IPM) (formula: $C_7H_{12}O_5$).



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	48	21	7	17	3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

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

Chain A: 70% 25% •

4 Data and refinement statistics (i)

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 21.04 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (6.00-2.00) 94.5 (21.04-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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)	0.39 , 257.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.58	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, MG, IPM

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	0.30	0/3260	0.56	0/4409

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3199	0	3223	109	50
2	A	12	0	8	0	0
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	38	1
All	All	3504	0	3266	109	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 (109) 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: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:231:GLY:C	6:A:2152:HOH:O	2.01	0.95
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:259:ASP:CG	1:A:260:GLY:H	1.77	0.86
1:A:415:ASN:CA	6:A:2223:HOH:O	2.10	0.84
1:A:80:GLN:OE1	6:A:2058:HOH:O	1.96	0.83
1:A:415:ASN:CG	6:A:2223:HOH:O	1.95	0.81
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:349:ASP:OD1	1:A:405:CYS:HB3	1.85	0.76
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:HB2	6:A:2056:HOH:O	1.91	0.71
1:A:138:PRO:HG3	1:A:393:PHE:O	1.93	0.68
1:A:259:ASP:CG	1:A:260:GLY:N	2.47	0.68
1:A:80:GLN:O	1:A:81:ASP:HB2	1.92	0.68
1:A:231:GLY:CA	6:A:2152:HOH:O	2.36	0.67
1:A:80:GLN:CD	6:A:2058:HOH:O	2.33	0.67
1:A:414:GLU:C	6:A:2223:HOH:O	2.09	0.65
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:80:GLN:CD	6:A:2056:HOH:O	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HG2	1:A:265:LYS:O	2.03	0.57
1:A:13:LYS:HE2	1:A:94:GLU:CG	2.35	0.57
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:341:THR:O	1:A:342:ALA:C	2.48	0.52
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: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:80:GLN:NE2	6:A:2056:HOH:O	2.45	0.48
1:A:73:LYS:HA	1:A:76:GLN:OE1	2.14	0.48
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:177:LYS:HZ2	1:A:181:GLU:CD	2.18	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:166:LYS:NZ	6:A:2112:HOH:O	2.32	0.46
1:A:33:GLU:HG2	6:A:2015:HOH:O	2.16	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:389:VAL:HG21	1:A:397:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HZ3	1:A:100:LYS:HG3	1.71	0.43
1:A:231:GLY:HA3	6:A:2152:HOH:O	2.14	0.43
1:A:389:VAL:HG21	1:A:397:MET:CE	2.48	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: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:17:GLN:NE2	1:A:22:ASN:HD22	2.17	0.42
1:A:221:ASP:CG	1:A:271:THR:HG21	2.38	0.42
1:A:326:ALA:HB2	1:A:335:PHE:CD2	2.54	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:167:ALA:O	1:A:168:ASP:HB2	2.20	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: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:135:GLN:CD	1:A:385:ASN:HD21	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	315 (94%)	21 (6%)	18 13

All (21) 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	132	ARG
1	A	135	GLN

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Mol	Chain	Res	Type
1	A	157	GLU
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	391	TYR
1	A	394	GLU
1	A	396	LEU
1	A	397	MET
1	A	404	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	288	GLN
1	A	316	GLN
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 monosaccharides 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	$\#\|Z\| > 2$
2	GOL	A	1418	-	5,5,5	4.37	4 (80%)	5,5,5	5.79	3 (60%)
3	IPM	A	1419	5	11,11,11	2.33	3 (27%)	10,15,15	1.41	3 (30%)
2	GOL	A	1417	-	5,5,5	4.36	4 (80%)	5,5,5	5.80	3 (60%)
4	NAP	A	1420	-	45,52,52	1.84	10 (22%)	56,80,80	1.53	12 (21%)

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	GOL	A	1418	-	-	2/4/4/4	-
3	IPM	A	1419	5	-	2/16/16/16	-
2	GOL	A	1417	-	-	2/4/4/4	-
4	NAP	A	1420	-	-	6/31/67/67	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1418	GOL	C3-C2	-7.39	1.21	1.51
2	A	1417	GOL	C3-C2	-7.35	1.21	1.51
4	A	1420	NAP	C2N-N1N	6.58	1.43	1.35
3	A	1419	IPM	O4-C4	4.77	1.36	1.22
2	A	1418	GOL	O1-C1	4.63	1.61	1.42
3	A	1419	IPM	O3-C1	4.60	1.36	1.22
2	A	1417	GOL	O1-C1	4.57	1.61	1.42
4	A	1420	NAP	C3N-C7N	-4.39	1.44	1.50
4	A	1420	NAP	C2A-N3A	4.33	1.39	1.32
2	A	1417	GOL	O3-C3	3.49	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1418	GOL	O3-C3	3.39	1.56	1.42
4	A	1420	NAP	C4A-N3A	3.37	1.40	1.35
4	A	1420	NAP	C6N-N1N	3.19	1.43	1.35
2	A	1417	GOL	O2-C2	-2.78	1.35	1.43
2	A	1418	GOL	O2-C2	-2.69	1.35	1.43
4	A	1420	NAP	P2B-O2B	2.52	1.64	1.59
4	A	1420	NAP	C8A-N7A	-2.42	1.30	1.34
4	A	1420	NAP	C4N-C3N	2.38	1.43	1.39
4	A	1420	NAP	C2N-C3N	2.27	1.42	1.39
4	A	1420	NAP	C5N-C4N	2.23	1.43	1.38
3	A	1419	IPM	C2-C1	2.04	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1417	GOL	O3-C3-C2	10.55	160.79	110.20
2	A	1418	GOL	O3-C3-C2	10.53	160.71	110.20
2	A	1417	GOL	O2-C2-C3	6.77	138.94	109.12
2	A	1418	GOL	O2-C2-C3	6.74	138.79	109.12
4	A	1420	NAP	N3A-C2A-N1A	-4.38	121.83	128.68
4	A	1420	NAP	C3B-C2B-C1B	-4.06	95.26	102.89
2	A	1418	GOL	O1-C1-C2	3.27	125.88	110.20
2	A	1417	GOL	O1-C1-C2	3.27	125.86	110.20
4	A	1420	NAP	C3N-C7N-N7N	2.93	121.27	117.75
4	A	1420	NAP	O5B-C5B-C4B	2.52	117.66	108.99
4	A	1420	NAP	O4B-C1B-C2B	-2.50	102.25	106.59
4	A	1420	NAP	O2N-PN-O1N	2.41	124.13	112.24
4	A	1420	NAP	C2A-N1A-C6A	2.39	122.84	118.75
3	A	1419	IPM	O2-C1-C2	2.35	119.63	113.27
4	A	1420	NAP	O4B-C4B-C3B	-2.32	100.52	105.11
4	A	1420	NAP	O3B-C3B-C4B	2.29	117.66	111.05
4	A	1420	NAP	O7N-C7N-N7N	-2.24	119.40	122.58
4	A	1420	NAP	O3B-C3B-C2B	2.06	117.02	111.17
3	A	1419	IPM	O5-C4-O4	-2.06	119.41	124.09
4	A	1420	NAP	PN-O5D-C5D	2.05	133.73	121.68
3	A	1419	IPM	O2-C1-O3	-2.01	119.52	124.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1417	GOL	O1-C1-C2-C3

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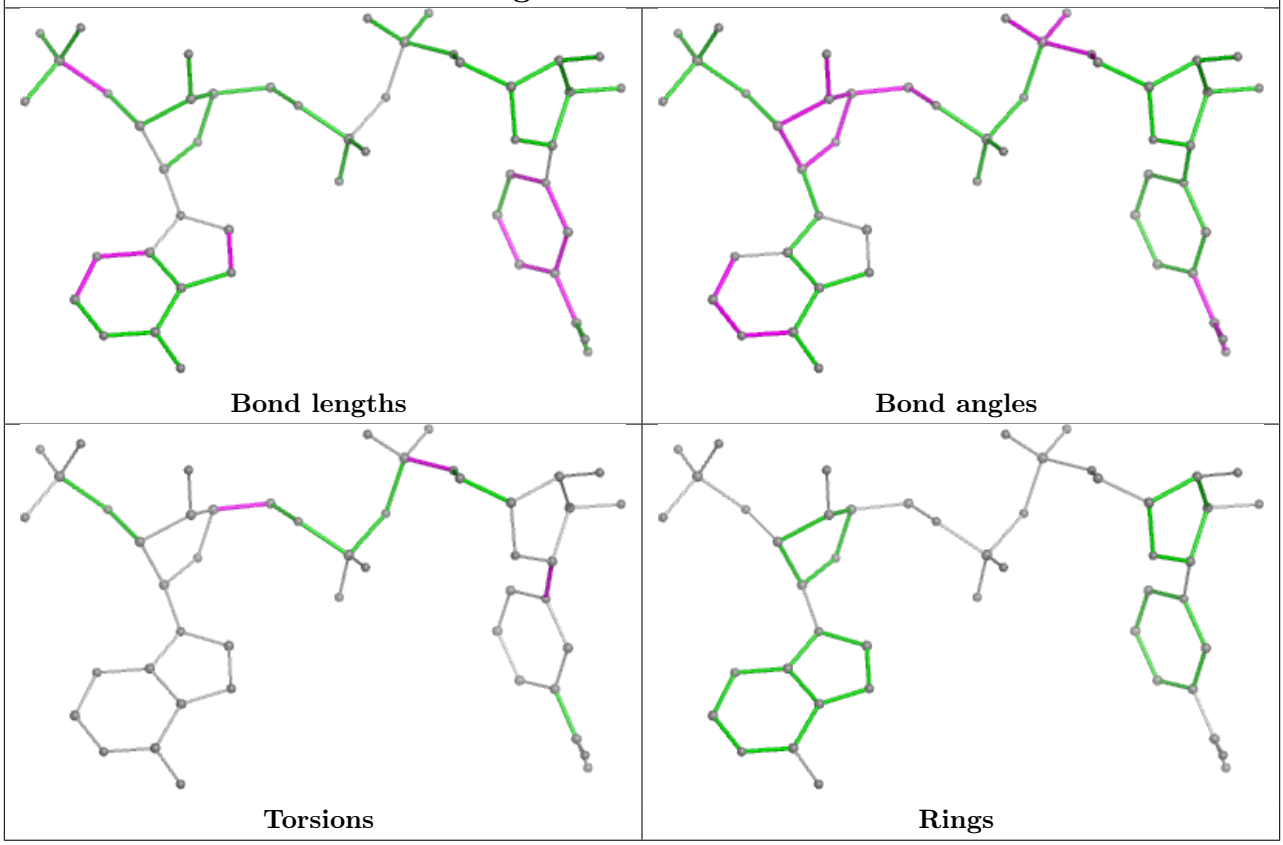
Mol	Chain	Res	Type	Atoms
2	A	1417	GOL	C1-C2-C3-O3
2	A	1418	GOL	O1-C1-C2-C3
2	A	1418	GOL	C1-C2-C3-O3
4	A	1420	NAP	O4D-C1D-N1N-C2N
4	A	1420	NAP	O4D-C1D-N1N-C6N
4	A	1420	NAP	O4B-C4B-C5B-O5B
4	A	1420	NAP	C3B-C4B-C5B-O5B
3	A	1419	IPM	C1-C2-C3-C4
4	A	1420	NAP	C5D-O5D-PN-O3
3	A	1419	IPM	C5-C3-C4-O5
4	A	1420	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAP A 1420



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

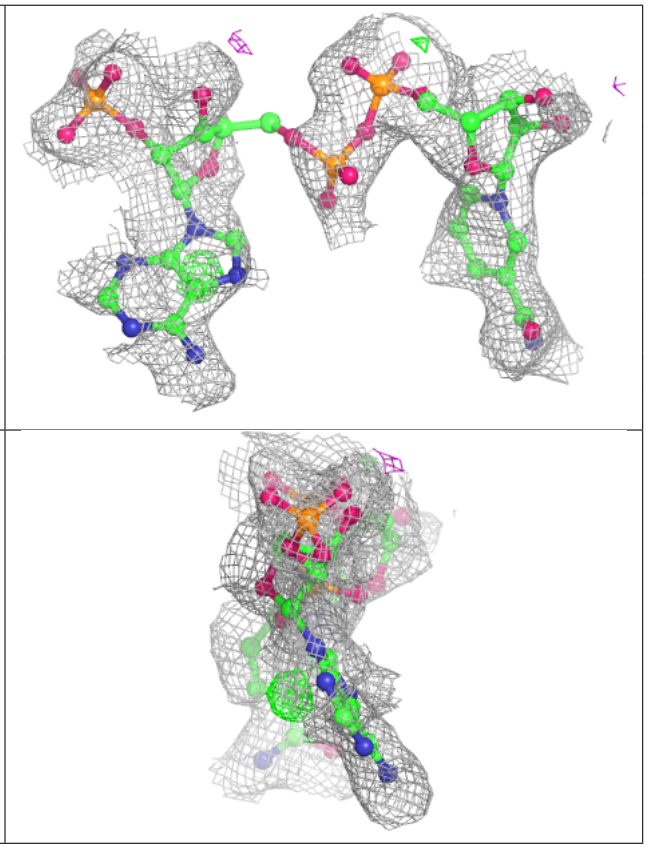
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP A 1420:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.