Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 05:06 PM EDT

PDB ID	:	1KOJ
Title	:	Crystal structure of rabbit phosphoglucose isomerase complexed with 5-phosp ho-D-arabinonohydroxamic acid
Authors	:	Arsenieva, D.; Hardre, R.; Salmon, L.; Jeffery, C.J.
Deposited on	:	2001-12-20
Resolution	:	1.90 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:

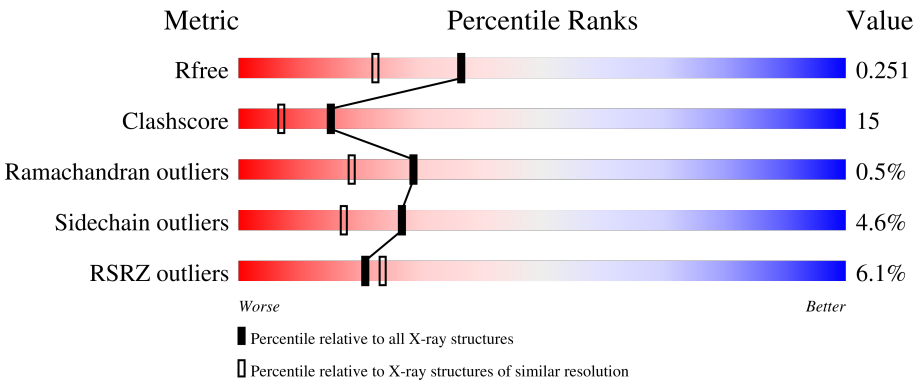
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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% 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	557	7% 71% 24% 5%
1	B	557	5% 76% 22% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9711 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.

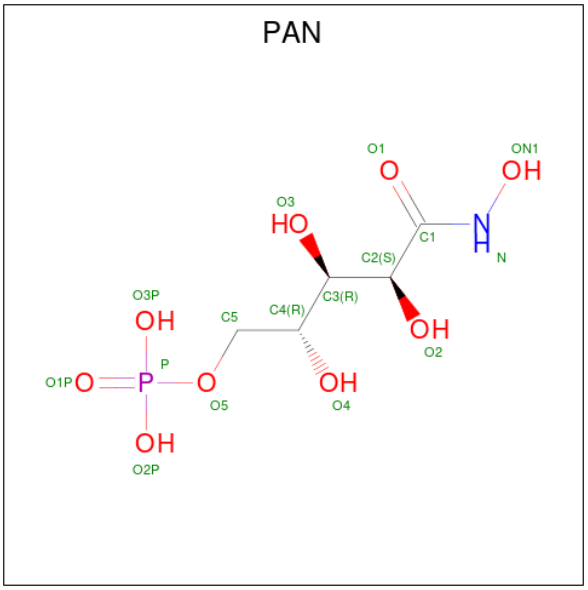
- Molecule 1 is a protein called Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4477	2859	779	820	19	0	10	0
1	B	556	4400	2808	766	807	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LYS	GLU	conflict	UNP Q9N1E2
B	222	LYS	GLU	conflict	UNP Q9N1E2

- Molecule 2 is 5-PHOSPHO-D-ARABINOHYDROXAMIC ACID (three-letter code: PAN) (formula: $C_5H_{12}NO_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	16	5	1	9	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	16	5	1	9	1	0	0

- Molecule 3 is water.

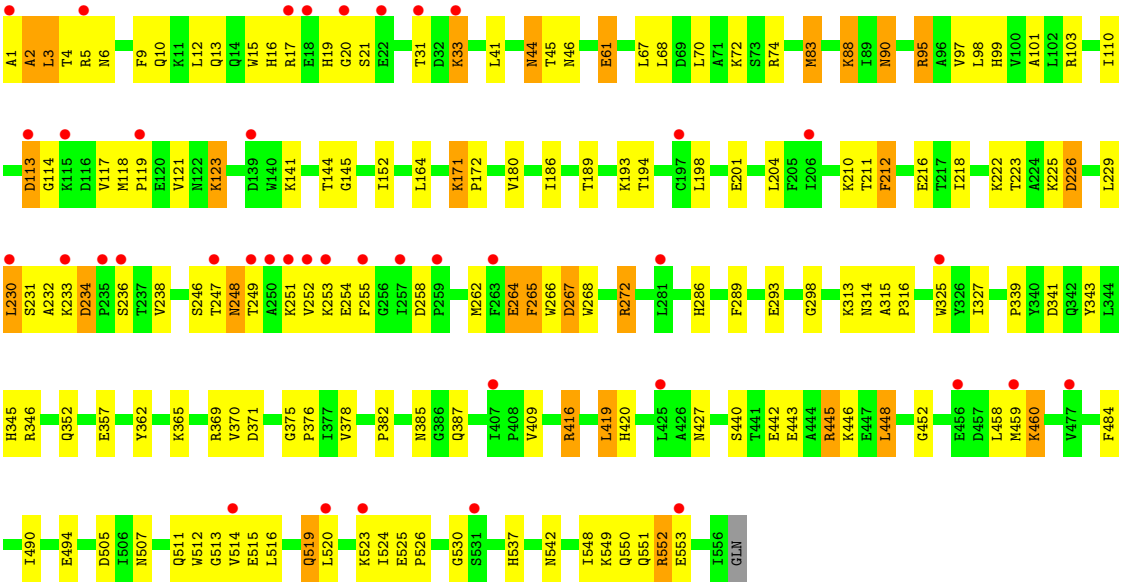
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	384	384	384	0	0
			Total	O		
3	B	418	418	418	0	0

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.

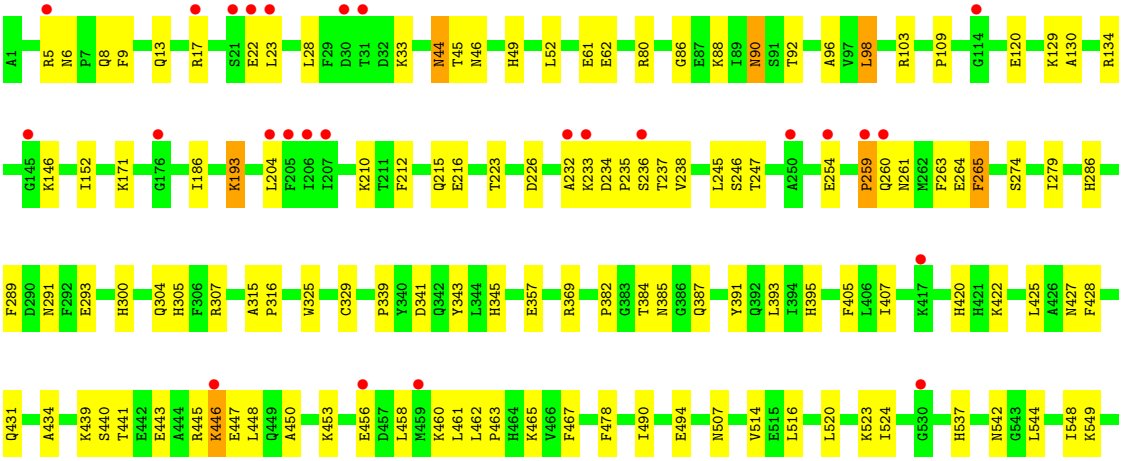
- Molecule 1: Glucose-6-phosphate isomerase

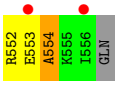
Chain A:



- Molecule 1: Glucose-6-phosphate isomerase

Chain B:




R552
E553
A554
K555
I556
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	82.69Å 115.97Å 271.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.90 24.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (12.00-1.90) 91.5 (24.05-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.254 0.218 , 0.251	Depositor DCC
R_{free} test set	9685 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9711	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: PAN

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	0.44	0/4588	0.68	5/6215 (0.1%)
1	B	0.41	0/4509	0.63	0/6108
All	All	0.42	0/9097	0.65	5/12323 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	552	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	A	272	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	95	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	A	369	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	83	MET	CG-SD-CE	6.17	110.07	100.20

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	4477	0	4432	173	0
1	B	4400	0	4354	107	0
2	A	16	0	10	1	0
2	B	16	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	384	0	0	19	0
3	B	418	0	0	19	0
All	All	9711	0	8806	266	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 15.

All (266) 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:327:ILE:HD11	1:A:376:PRO:HG3	1.35	1.06
1:A:416:ARG:HH11	1:A:416:ARG:HB3	1.17	1.06
1:B:548:ILE:HG23	3:B:1270:HOH:O	1.56	1.05
1:A:95:ARG:HD3	1:A:267:ASP:HB2	1.41	1.02
1:A:409:VAL:HG13	3:B:1270:HOH:O	1.59	1.02
1:A:416:ARG:HH12	1:A:419:LEU:HD12	1.24	0.99
1:B:28:LEU:HD11	3:B:1272:HOH:O	1.60	0.99
1:A:516[B]:LEU:HD13	1:B:434:ALA:HB1	1.46	0.94
1:A:549:LYS:HA	1:A:552:ARG:CD	1.97	0.93
1:B:120:GLU:HG2	3:B:1206:HOH:O	1.77	0.85
1:A:549:LYS:HA	1:A:552:ARG:HD2	1.58	0.84
1:B:446:LYS:C	1:B:446:LYS:HD3	1.97	0.84
1:A:12:LEU:HD11	1:A:67:LEU:HD23	1.63	0.80
1:B:305:HIS:HE1	1:B:315:ALA:H	1.24	0.79
1:B:453:LYS:HE2	1:B:461:LEU:HD13	1.63	0.79
1:A:211:THR:O	1:A:251:LYS:HD2	1.83	0.78
1:A:225:LYS:HE3	1:A:238:VAL:HG21	1.66	0.78
1:B:23:LEU:HD22	3:B:1272:HOH:O	1.84	0.77
1:A:315:ALA:HB3	1:A:316:PRO:HD3	1.67	0.76
1:B:537:HIS:H	1:B:542:ASN:HD21	1.33	0.76
1:A:537:HIS:H	1:A:542:ASN:HD21	1.30	0.76
1:B:6:ASN:HD21	1:B:8:GLN:HB2	1.49	0.76
1:A:110:ILE:HD12	1:A:118:MET:HE3	1.68	0.75
1:B:238:VAL:HG23	3:B:1292:HOH:O	1.87	0.75
1:B:193:LYS:HE3	1:B:193:LYS:HA	1.68	0.74
1:A:2:ALA:O	1:A:5:ARG:HG2	1.88	0.74
1:A:550:GLN:HE21	1:A:551:GLN:HE21	1.33	0.74
1:A:549:LYS:HA	1:A:552:ARG:HD3	1.71	0.72
1:A:525:GLU:HG2	1:B:422:LYS:HE2	1.71	0.70
1:B:516:LEU:HD11	1:B:520:LEU:HD21	1.74	0.69
1:A:416:ARG:HH11	1:A:416:ARG:CB	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:HB1	1:A:118:MET:HE1	1.76	0.68
1:A:327:ILE:CD1	1:A:376:PRO:HG3	2.17	0.67
1:B:461:LEU:HD21	1:B:465:LYS:HD2	1.76	0.67
1:B:441:THR:HG23	1:B:462:LEU:HD11	1.75	0.67
1:A:41:LEU:HD12	1:A:41:LEU:O	1.94	0.67
1:A:416:ARG:HB3	1:A:416:ARG:NH1	2.02	0.66
1:A:548:ILE:HD13	1:B:425:LEU:HD22	1.78	0.66
1:A:83:MET:CE	1:A:97:VAL:HG12	2.27	0.65
1:B:109:PRO:HG2	3:B:1061:HOH:O	1.96	0.64
1:A:515[B]:GLU:O	1:A:519[B]:GLN:HG3	1.97	0.64
1:A:514[B]:VAL:HG23	1:A:514[B]:VAL:O	1.98	0.64
1:A:88:LYS:HB2	1:A:88:LYS:NZ	2.13	0.64
1:A:83:MET:HE3	1:A:97:VAL:CG1	2.28	0.64
1:B:259:PRO:O	1:B:260:GLN:HB3	1.96	0.64
1:B:345:HIS:HA	1:B:382:PRO:HG3	1.80	0.64
1:A:248:ASN:HB3	1:A:251:LYS:HG2	1.79	0.63
1:A:416:ARG:NH1	1:A:419:LEU:HD12	2.05	0.63
1:A:144:THR:HG21	1:A:201:GLU:CD	2.19	0.63
1:A:387:GLN:HE22	1:A:427:ASN:HB3	1.64	0.63
1:A:45:THR:O	1:A:46:ASN:HB2	1.98	0.63
1:A:83:MET:CE	1:A:99:HIS:CE1	2.81	0.63
1:A:314:ASN:OD1	1:A:316:PRO:HD2	1.98	0.62
1:A:520[B]:LEU:HD22	1:A:523:LYS:HE3	1.81	0.62
1:B:44:ASN:ND2	1:B:46:ASN:H	1.97	0.62
1:B:461:LEU:HD21	1:B:465:LYS:CD	2.29	0.62
1:A:83:MET:HE1	1:A:99:HIS:CE1	2.36	0.61
1:B:254:GLU:HG2	3:B:1237:HOH:O	1.99	0.61
1:B:289:PHE:O	1:B:293:GLU:HG3	2.00	0.61
1:B:259:PRO:C	1:B:261:ASN:H	2.04	0.61
1:B:17:ARG:HG2	3:B:1260:HOH:O	2.01	0.60
1:A:74:ARG:HH11	1:A:74:ARG:HA	1.67	0.60
1:B:6:ASN:ND2	1:B:8:GLN:HB2	2.17	0.60
1:B:90:ASN:ND2	1:B:507:ASN:HD21	2.00	0.60
1:A:511:GLN:O	1:A:515[A]:GLU:HG2	2.00	0.60
1:A:513[B]:GLY:HA2	1:B:467:PHE:CZ	2.36	0.60
1:B:305:HIS:CE1	1:B:315:ALA:H	2.14	0.60
1:A:123:LYS:HE2	3:A:1240:HOH:O	2.02	0.59
1:A:223:THR:OG1	1:B:420:HIS:HE1	1.85	0.59
1:A:520[B]:LEU:O	1:A:523:LYS:HG2	2.03	0.59
1:A:511:GLN:O	1:A:514[B]:VAL:HG13	2.03	0.58
1:B:6:ASN:HD22	1:B:9:PHE:H	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LYS:HA	1:B:193:LYS:CE	2.32	0.58
1:B:61:GLU:HG2	3:B:1246:HOH:O	2.04	0.58
1:A:90:ASN:ND2	1:A:507:ASN:HD21	2.01	0.57
1:A:549:LYS:O	1:A:552:ARG:HG2	2.04	0.57
1:A:234:ASP:C	1:A:236:SER:H	2.05	0.57
1:A:409:VAL:HG22	1:B:548:ILE:HD13	1.85	0.57
1:A:289:PHE:O	1:A:293:GLU:HG3	2.03	0.57
1:A:2:ALA:HB2	3:A:1013:HOH:O	2.03	0.57
1:A:248:ASN:O	1:A:252:VAL:HG23	2.05	0.57
1:A:513[B]:GLY:HA2	1:B:467:PHE:CE2	2.39	0.57
1:B:246:SER:O	1:B:264:GLU:HA	2.05	0.57
1:A:68:LEU:O	1:A:72:LYS:HG2	2.05	0.56
1:A:523:LYS:HZ3	1:A:524:ILE:HG13	1.71	0.56
1:A:44:ASN:ND2	1:A:46:ASN:H	2.04	0.56
1:B:462:LEU:HB3	1:B:463:PRO:HD3	1.87	0.56
1:A:193:LYS:HE3	3:A:1163:HOH:O	2.04	0.56
1:A:460:LYS:HE3	1:A:460:LYS:O	2.06	0.56
1:B:235:PRO:O	1:B:238:VAL:HG22	2.06	0.56
1:A:83:MET:HE2	1:A:97:VAL:HG12	1.88	0.56
1:A:114:GLY:HA3	3:A:1121:HOH:O	2.05	0.56
1:B:22:GLU:O	1:B:23:LEU:HG	2.06	0.56
1:A:249:THR:HA	1:A:262:MET:SD	2.45	0.56
1:B:445:ARG:HG3	1:B:458:LEU:HD21	1.87	0.55
1:A:365:LYS:HB2	3:A:1129:HOH:O	2.07	0.55
1:A:549:LYS:O	1:A:552:ARG:CG	2.54	0.55
1:A:327:ILE:HD11	1:A:376:PRO:CG	2.24	0.55
1:B:369:ARG:HG2	1:B:369:ARG:HH11	1.71	0.55
1:B:445:ARG:HG2	1:B:445:ARG:HH11	1.70	0.55
1:A:118:MET:N	1:A:119:PRO:HD2	2.21	0.55
1:B:129:LYS:HD3	3:B:1199:HOH:O	2.07	0.55
1:A:68:LEU:O	1:A:72:LYS:HE2	2.06	0.55
1:B:387:GLN:HE22	1:B:427:ASN:HB3	1.72	0.54
1:A:33:LYS:N	1:A:33:LYS:HD2	2.22	0.54
1:A:83:MET:HE3	1:A:97:VAL:HG12	1.89	0.54
1:A:246:SER:O	1:A:264:GLU:HA	2.07	0.54
1:A:512[B]:TRP:HZ3	3:A:1130:HOH:O	1.90	0.53
1:B:6:ASN:ND2	1:B:8:GLN:H	2.06	0.53
1:A:490:ILE:O	1:A:494:GLU:HG3	2.08	0.53
1:A:516[A]:LEU:O	1:A:520[A]:LEU:HG	2.08	0.53
1:A:141:LYS:CG	1:A:145:GLY:HA2	2.39	0.53
1:A:193:LYS:CE	3:A:1163:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:MET:HE3	1:A:97:VAL:HG11	1.90	0.53
1:A:519[B]:GLN:HE22	1:B:439:LYS:NZ	2.06	0.53
3:A:1067:HOH:O	1:B:49:HIS:HD2	1.91	0.53
1:A:6:ASN:O	1:A:10:GLN:HG3	2.09	0.52
1:B:461:LEU:C	1:B:461:LEU:HD23	2.30	0.52
1:A:88:LYS:HB2	1:A:88:LYS:HZ2	1.74	0.52
1:A:345:HIS:HA	1:A:382:PRO:HG3	1.90	0.52
1:A:152:ILE:HD12	1:A:152:ILE:N	2.24	0.52
1:A:225:LYS:O	1:A:229:LEU:HD13	2.10	0.51
1:B:524:ILE:HG13	3:B:1036:HOH:O	2.11	0.51
1:A:180:VAL:HG21	1:A:286:HIS:HB2	1.91	0.51
1:B:544:LEU:O	1:B:548:ILE:HG12	2.11	0.51
1:A:171:LYS:HE2	3:A:1139:HOH:O	2.10	0.51
1:B:90:ASN:C	1:B:90:ASN:HD22	2.12	0.51
1:A:516[A]:LEU:HG	1:A:520[A]:LEU:HD21	1.93	0.50
1:B:45:THR:O	1:B:46:ASN:HB2	2.12	0.50
1:A:341:ASP:OD2	1:A:343:TYR:HB2	2.11	0.50
1:A:515[B]:GLU:OE2	3:A:1203:HOH:O	2.20	0.50
1:A:15:TRP:O	1:A:19:HIS:HB2	2.12	0.50
1:A:1:ALA:HB2	1:A:371:ASP:HB2	1.93	0.50
1:A:31:THR:O	1:A:31:THR:HG22	2.11	0.50
1:A:74:ARG:HA	1:A:74:ARG:NH1	2.26	0.50
1:A:420:HIS:HE1	1:B:223:THR:OG1	1.93	0.50
1:A:61:GLU:H	1:A:61:GLU:CD	2.15	0.50
1:A:70:LEU:O	1:A:70:LEU:HD23	2.11	0.50
1:B:490:ILE:O	1:B:494:GLU:HG3	2.11	0.49
1:A:13:GLN:HG2	3:A:1033:HOH:O	2.12	0.49
1:A:16:HIS:CD2	1:A:20:GLY:HA3	2.47	0.49
1:A:440:SER:OG	1:A:443:GLU:HG3	2.11	0.49
1:A:95:ARG:HD3	1:A:267:ASP:CB	2.29	0.49
1:B:549:LYS:HG2	1:B:552:ARG:NH2	2.27	0.49
1:A:210:LYS:HA	1:A:265:PHE:CZ	2.48	0.49
1:A:458:LEU:C	1:A:458:LEU:HD23	2.32	0.49
1:A:2:ALA:HA	1:A:5:ARG:HD3	1.95	0.49
1:A:232:ALA:O	1:A:233:LYS:HB2	2.12	0.49
1:B:234:ASP:HB3	1:B:237:THR:HG23	1.93	0.49
1:A:226:ASP:O	1:A:230:LEU:HG	2.12	0.49
1:A:452:GLY:C	3:A:1120:HOH:O	2.50	0.49
1:A:251:LYS:HA	1:A:254:GLU:HG2	1.95	0.49
1:B:146:LYS:HE3	3:B:1081:HOH:O	2.12	0.49
1:B:171:LYS:HD3	1:B:286:HIS:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:CE	1:A:238:VAL:HG21	2.40	0.49
1:A:512[B]:TRP:O	1:B:467:PHE:HZ	1.96	0.49
1:B:232:ALA:O	1:B:233:LYS:HB2	2.13	0.48
1:B:516:LEU:CD1	1:B:520:LEU:HD21	2.42	0.48
1:B:325:TRP:O	1:B:329:CYS:HB2	2.14	0.48
1:A:189:THR:O	1:A:193:LYS:HG2	2.13	0.48
1:A:12:LEU:HD12	1:A:70:LEU:HD12	1.96	0.48
1:A:83:MET:HE2	1:A:99:HIS:CE1	2.49	0.48
1:A:90:ASN:C	1:A:90:ASN:HD22	2.16	0.48
1:A:152:ILE:HG12	1:A:198:LEU:HD21	1.95	0.48
1:A:520[B]:LEU:HD22	1:A:523:LYS:CE	2.44	0.47
1:A:164:LEU:HD11	1:A:346:ARG:HG3	1.96	0.47
1:A:164:LEU:HD13	1:A:164:LEU:C	2.35	0.47
1:A:264:GLU:OE1	1:A:266:TRP:CE2	2.66	0.47
1:A:357:GLU:OE1	1:A:514[A]:VAL:HG21	2.15	0.47
1:A:409:VAL:HG22	1:B:548:ILE:CD1	2.44	0.47
1:A:41:LEU:HD12	1:A:41:LEU:C	2.34	0.47
1:A:141:LYS:HG2	1:A:145:GLY:HA2	1.95	0.47
1:B:245:LEU:HA	1:B:263:PHE:O	2.15	0.47
1:A:194:THR:O	1:A:198:LEU:HD13	2.15	0.47
1:A:234:ASP:C	1:A:236:SER:N	2.68	0.46
1:B:341:ASP:OD2	1:B:343:TYR:HB2	2.15	0.46
1:B:407:ILE:HD13	1:B:425:LEU:HD23	1.97	0.46
1:A:95:ARG:CD	1:A:267:ASP:HB2	2.29	0.46
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.50	0.46
1:A:117:VAL:O	1:A:121:VAL:HG23	2.14	0.46
1:B:387:GLN:HA	1:B:391:TYR:CG	2.50	0.46
1:A:110:ILE:HD12	1:A:118:MET:CE	2.41	0.46
1:A:204:LEU:C	1:A:204:LEU:HD23	2.36	0.46
1:A:460:LYS:HE2	1:B:92:THR:HA	1.96	0.46
1:A:123:LYS:HA	1:A:123:LYS:HD2	1.83	0.46
1:B:300:HIS:O	1:B:304:GLN:HG3	2.16	0.46
1:A:375:GLY:O	1:B:393:LEU:HD11	2.15	0.45
1:B:446:LYS:HD3	1:B:447:GLU:N	2.29	0.45
1:A:4:THR:OG1	1:A:371:ASP:HB3	2.16	0.45
1:B:395:HIS:HE1	1:B:431:GLN:OE1	1.99	0.45
1:B:260:GLN:HA	1:B:260:GLN:HE21	1.81	0.45
1:B:357:GLU:OE1	1:B:514:VAL:HG21	2.17	0.45
1:B:232:ALA:HB1	1:B:237:THR:OG1	2.15	0.45
1:B:384:THR:O	1:B:385:ASN:C	2.55	0.45
1:A:171:LYS:N	1:A:172:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:TYR:O	1:A:370:VAL:HG22	2.17	0.45
1:B:52:LEU:HB2	3:B:1106:HOH:O	2.15	0.45
1:A:83:MET:HE2	3:A:918:HOH:O	2.17	0.45
1:B:274:SER:O	1:B:279:ILE:HB	2.17	0.45
1:B:186:ILE:HB	1:B:216:GLU:HG3	1.98	0.44
1:B:305:HIS:HE1	1:B:315:ALA:N	2.04	0.44
1:A:141:LYS:HD2	1:A:145:GLY:O	2.18	0.44
1:A:247:THR:HG22	1:A:265:PHE:O	2.17	0.44
1:B:448:LEU:HD21	1:B:465:LYS:HD3	2.00	0.44
1:A:12:LEU:HD22	1:A:325:TRP:CZ3	2.53	0.44
1:A:313:LYS:HB3	1:A:313:LYS:HE3	1.67	0.44
1:B:259:PRO:C	1:B:261:ASN:N	2.71	0.44
1:B:210:LYS:HA	1:B:265:PHE:CZ	2.53	0.44
1:A:3:LEU:HD22	1:A:9:PHE:CD1	2.52	0.44
1:A:460:LYS:HE3	1:A:460:LYS:C	2.38	0.43
1:B:458:LEU:HD23	1:B:458:LEU:C	2.39	0.43
1:A:212:PHE:O	1:A:218:ILE:HD11	2.19	0.43
1:A:13:GLN:O	1:A:17:ARG:HB2	2.19	0.43
1:A:459:MET:HE1	3:B:1209:HOH:O	2.17	0.43
1:A:552:ARG:HD3	3:A:1077:HOH:O	2.17	0.43
1:A:193:LYS:NZ	3:A:1163:HOH:O	2.51	0.43
1:B:456:GLU:HG2	3:B:1201:HOH:O	2.17	0.43
1:A:234:ASP:O	1:A:236:SER:N	2.51	0.43
1:B:247:THR:HG22	1:B:265:PHE:O	2.18	0.43
1:B:548:ILE:HD13	1:B:548:ILE:HA	1.88	0.43
1:A:253:LYS:C	1:A:255:PHE:H	2.21	0.43
1:A:90:ASN:HB3	1:A:95:ARG:O	2.18	0.43
1:B:152:ILE:N	1:B:152:ILE:HD12	2.34	0.43
1:B:204:LEU:C	1:B:204:LEU:HD13	2.39	0.43
1:B:315:ALA:HB3	1:B:316:PRO:CD	2.49	0.43
1:A:445:ARG:NH2	3:A:1265:HOH:O	2.53	0.42
1:A:117:VAL:HG23	1:A:118:MET:HE1	2.01	0.42
1:A:141:LYS:HG3	1:A:145:GLY:HA2	2.00	0.42
1:B:446:LYS:HE3	1:B:450:ALA:HB2	2.00	0.42
1:A:70:LEU:HD23	1:A:70:LEU:C	2.39	0.42
1:A:212:PHE:CD1	1:A:252:VAL:HG22	2.55	0.42
1:B:88:LYS:HA	1:B:96:ALA:HA	2.00	0.42
1:B:215:GLN:NE2	3:B:952:HOH:O	2.53	0.42
1:A:21:SER:HB2	3:A:1177:HOH:O	2.18	0.42
1:A:272:ARG:HG2	2:A:902:PAN:ON1	2.19	0.42
1:A:365:LYS:HD3	3:A:1129:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLN:HA	1:A:378:VAL:HB	2.02	0.42
1:B:440:SER:OG	1:B:443:GLU:HG3	2.19	0.41
1:A:265:PHE:N	1:A:265:PHE:CD2	2.88	0.41
1:B:553:GLU:O	1:B:554:ALA:C	2.58	0.41
1:A:448:LEU:HB3	1:A:458:LEU:HG	2.03	0.41
1:B:23:LEU:CD2	3:B:1272:HOH:O	2.58	0.41
1:A:212:PHE:CG	1:A:252:VAL:HG22	2.55	0.41
1:A:327:ILE:HD13	1:A:376:PRO:HD3	2.03	0.41
1:A:3:LEU:HD22	1:A:9:PHE:CG	2.55	0.41
1:A:548:ILE:O	1:A:552:ARG:HG2	2.20	0.41
1:B:13:GLN:O	1:B:17:ARG:HG3	2.20	0.41
1:B:385:ASN:ND2	3:B:990:HOH:O	2.53	0.41
1:A:442:GLU:O	1:A:446:LYS:HG3	2.21	0.41
1:A:101:ALA:HB1	1:A:118:MET:CE	2.47	0.41
1:A:525:GLU:N	1:A:526:PRO:HD2	2.36	0.41
1:A:98:LEU:HB2	1:A:268:TRP:CE3	2.56	0.41
1:A:298:GLY:HA3	1:A:484:PHE:O	2.20	0.41
1:A:505:ASP:CG	3:A:1129:HOH:O	2.59	0.41
1:B:6:ASN:ND2	1:B:8:GLN:N	2.68	0.41
1:B:86:GLY:HA2	1:B:98:LEU:HD11	2.02	0.41
1:A:420:HIS:HD2	1:B:186:ILE:O	2.04	0.41
1:B:80:ARG:HD2	1:B:307:ARG:HA	2.02	0.41
1:A:246:SER:OG	1:A:247:THR:N	2.53	0.40
1:A:186:ILE:HB	1:A:216:GLU:HG3	2.03	0.40
1:A:530:GLY:O	1:A:552:ARG:NH1	2.55	0.40
1:B:369:ARG:HG2	1:B:369:ARG:NH1	2.35	0.40
1:A:339:PRO:O	1:A:382:PRO:HA	2.22	0.40
1:B:130:ALA:O	1:B:134:ARG:HG3	2.22	0.40
1:A:519[A]:GLN:CA	1:A:519[A]:GLN:NE2	2.82	0.40
1:B:291:ASN:HD22	1:B:291:ASN:HA	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/557 (101%)	522 (93%)	38 (7%)	4 (1%)	22	12
1	B	554/557 (100%)	523 (94%)	29 (5%)	2 (0%)	34	24
All	All	1118/1114 (100%)	1045 (94%)	67 (6%)	6 (0%)	29	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	113	ASP
1	A	385	ASN
1	B	554	ALA
1	A	234	ASP
1	B	259	PRO

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	482/478 (101%)	454 (94%)	28 (6%)	20	10
1	B	475/478 (99%)	458 (96%)	17 (4%)	35	26
All	All	957/956 (100%)	912 (95%)	45 (5%)	27	16

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	33	LYS
1	A	44	ASN
1	A	61	GLU
1	A	88	LYS
1	A	90	ASN
1	A	103	ARG

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Mol	Chain	Res	Type
1	A	113	ASP
1	A	123	LYS
1	A	171	LYS
1	A	212	PHE
1	A	222	LYS
1	A	226	ASP
1	A	230	LEU
1	A	231	SER
1	A	248	ASN
1	A	258	ASP
1	A	264	GLU
1	A	265	PHE
1	A	267	ASP
1	A	416	ARG
1	A	419	LEU
1	A	445	ARG
1	A	448	LEU
1	A	460	LYS
1	A	519[A]	GLN
1	A	519[B]	GLN
1	A	553	GLU
1	B	5	ARG
1	B	33	LYS
1	B	44	ASN
1	B	62	GLU
1	B	90	ASN
1	B	98	LEU
1	B	103	ARG
1	B	193	LYS
1	B	212	PHE
1	B	226	ASP
1	B	236	SER
1	B	265	PHE
1	B	339	PRO
1	B	446	LYS
1	B	460	LYS
1	B	478	PHE
1	B	523	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	46	ASN
1	A	90	ASN
1	A	133	GLN
1	A	153	ASN
1	A	215	GLN
1	A	387	GLN
1	A	420	HIS
1	A	542	ASN
1	A	550	GLN
1	B	6	ASN
1	B	13	GLN
1	B	44	ASN
1	B	46	ASN
1	B	49	HIS
1	B	90	ASN
1	B	107	ASN
1	B	153	ASN
1	B	215	GLN
1	B	260	GLN
1	B	286	HIS
1	B	291	ASN
1	B	304	GLN
1	B	305	HIS
1	B	359	ASN
1	B	387	GLN
1	B	395	HIS
1	B	410	GLN
1	B	420	HIS
1	B	431	GLN
1	B	449	GLN
1	B	542	ASN
1	B	550	GLN
1	B	551	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	PAN	A	902	-	15,15,15	1.61	3 (20%)	19,21,21	3.21	7 (36%)
2	PAN	B	901	-	15,15,15	1.61	3 (20%)	19,21,21	3.21	7 (36%)

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	PAN	A	902	-	-	0/20/20/20	-
2	PAN	B	901	-	-	0/20/20/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	PAN	C5-C4	3.65	1.57	1.51
2	B	901	PAN	C5-C4	3.60	1.56	1.51
2	B	901	PAN	ON1-N	2.39	1.46	1.40
2	A	902	PAN	ON1-N	2.37	1.46	1.40
2	B	901	PAN	C2-C1	2.13	1.57	1.52
2	A	902	PAN	C2-C1	2.10	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	PAN	O1-C1-C2	7.83	134.12	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	902	PAN	O1-C1-C2	7.83	134.11	120.00
2	B	901	PAN	C2-C1-N	-7.33	106.98	116.19
2	A	902	PAN	C2-C1-N	-7.31	107.01	116.19
2	B	901	PAN	O2-C2-C1	4.14	119.54	110.63
2	A	902	PAN	O2-C2-C1	4.13	119.53	110.63
2	B	901	PAN	P-O5-C5	-3.62	108.31	118.30
2	A	902	PAN	P-O5-C5	-3.61	108.34	118.30
2	A	902	PAN	O1-C1-N	-3.39	118.88	123.27
2	B	901	PAN	O1-C1-N	-3.38	118.90	123.27
2	B	901	PAN	C3-C2-C1	-3.37	101.72	109.91
2	A	902	PAN	C3-C2-C1	-3.36	101.73	109.91
2	A	902	PAN	C5-C4-C3	-2.74	106.91	112.20
2	B	901	PAN	C5-C4-C3	-2.73	106.93	112.20

There are no chirality outliers.

There are no torsion outliers.

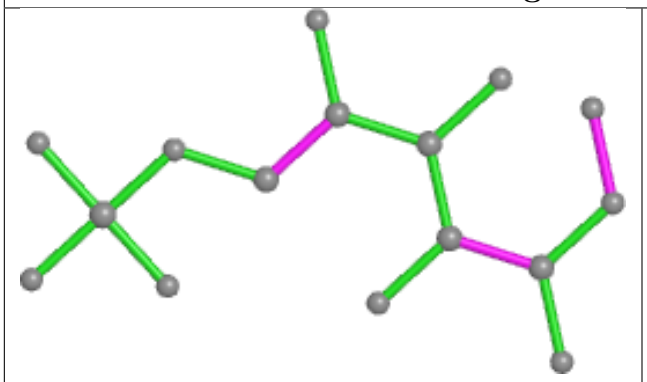
There are no ring outliers.

1 monomer is involved in 1 short contact:

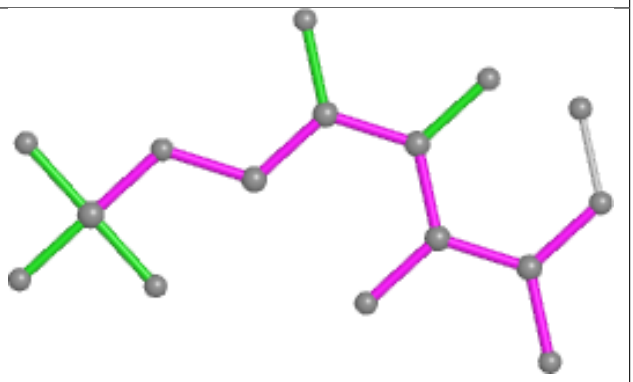
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	PAN	1	0

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 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.

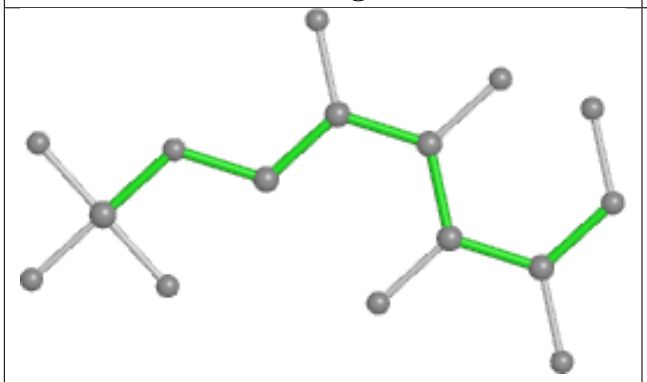
Ligand PAN A 902



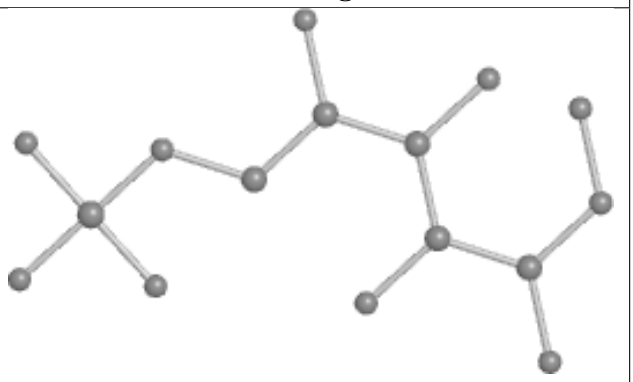
Bond lengths



Bond angles

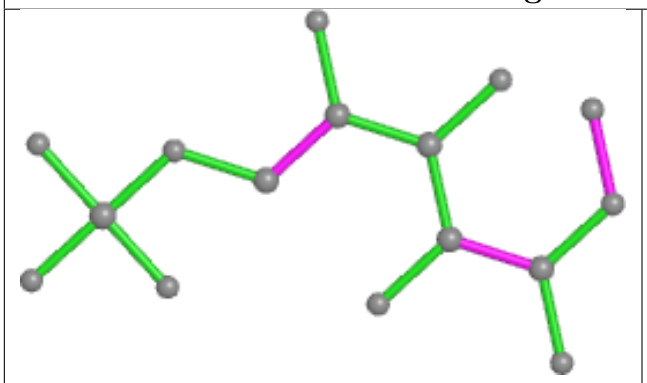


Torsions

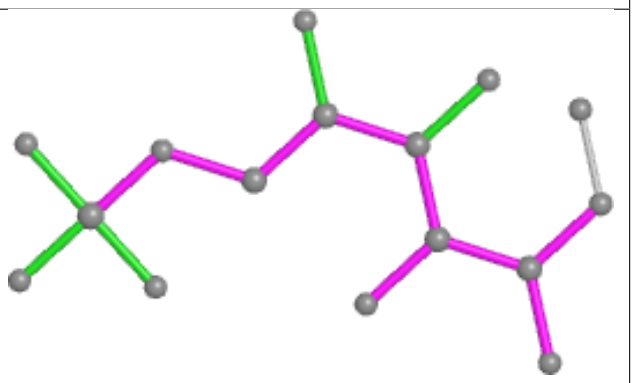


Rings

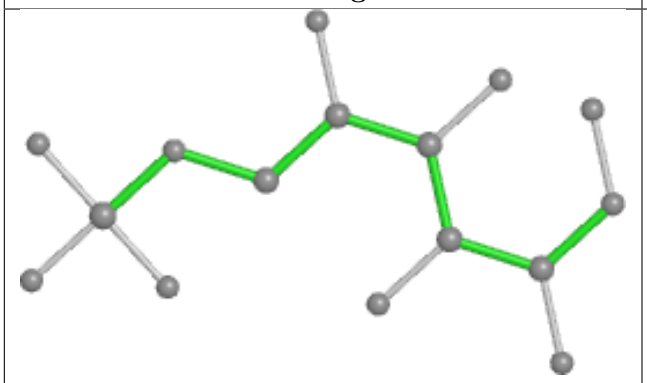
Ligand PAN B 901



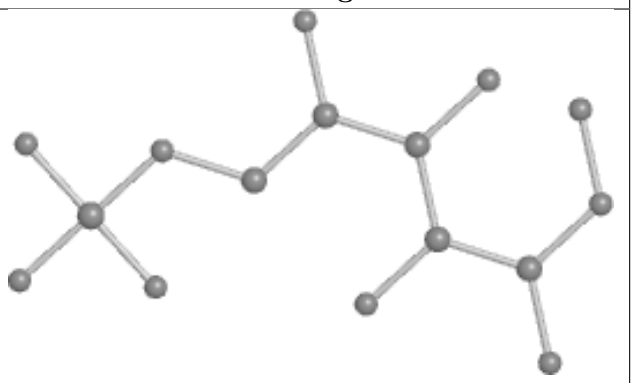
Bond lengths



Bond angles



Torsions



Rings

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)

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	556/557 (99%)	0.44	40 (7%)	15	17	26, 43, 71, 87	0
1	B	556/557 (99%)	0.35	28 (5%)	28	32	26, 39, 63, 74	0
All	All	1112/1114 (99%)	0.40	68 (6%)	21	24	26, 40, 67, 87	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	GLY	6.2
1	A	235	PRO	4.9
1	A	113	ASP	4.8
1	B	114	GLY	4.6
1	A	206	ILE	4.4
1	A	247	THR	4.1
1	A	1	ALA	4.0
1	B	206	ILE	4.0
1	A	197	CYS	4.0
1	A	230	LEU	3.8
1	B	236	SER	3.8
1	A	257	ILE	3.7
1	A	456	GLU	3.6
1	B	21	SER	3.5
1	B	5	ARG	3.3
1	B	250	ALA	3.3
1	B	556	ILE	3.3
1	A	259	PRO	3.2
1	B	145	GLY	3.2
1	A	255	PHE	3.2
1	B	22	GLU	3.1
1	A	5	ARG	3.1
1	A	252	VAL	3.0
1	A	281	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	456	GLU	3.0
1	A	520[A]	LEU	2.9
1	A	236	SER	2.9
1	A	17	ARG	2.9
1	B	233	LYS	2.9
1	A	18	GLU	2.8
1	A	31	THR	2.8
1	A	115	LYS	2.8
1	A	22	GLU	2.8
1	B	260	GLN	2.7
1	A	553	GLU	2.7
1	A	249	THR	2.7
1	A	514[A]	VAL	2.6
1	B	254	GLU	2.5
1	A	139	ASP	2.5
1	B	259	PRO	2.5
1	A	253	LYS	2.5
1	A	119	PRO	2.5
1	A	233	LYS	2.4
1	B	207	ILE	2.4
1	B	204	LEU	2.4
1	A	459	MET	2.4
1	B	23	LEU	2.3
1	B	205	PHE	2.3
1	A	407	ILE	2.3
1	A	33	LYS	2.3
1	A	425	LEU	2.3
1	B	417	LYS	2.3
1	B	553	GLU	2.3
1	B	17	ARG	2.3
1	B	459	MET	2.2
1	A	251	LYS	2.2
1	B	176	GLY	2.2
1	A	523	LYS	2.2
1	A	263	PHE	2.1
1	A	531	SER	2.1
1	B	530	GLY	2.1
1	B	232	ALA	2.1
1	B	446	LYS	2.1
1	B	30	ASP	2.1
1	A	477	VAL	2.0
1	A	250	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	325	TRP	2.0
1	B	31	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

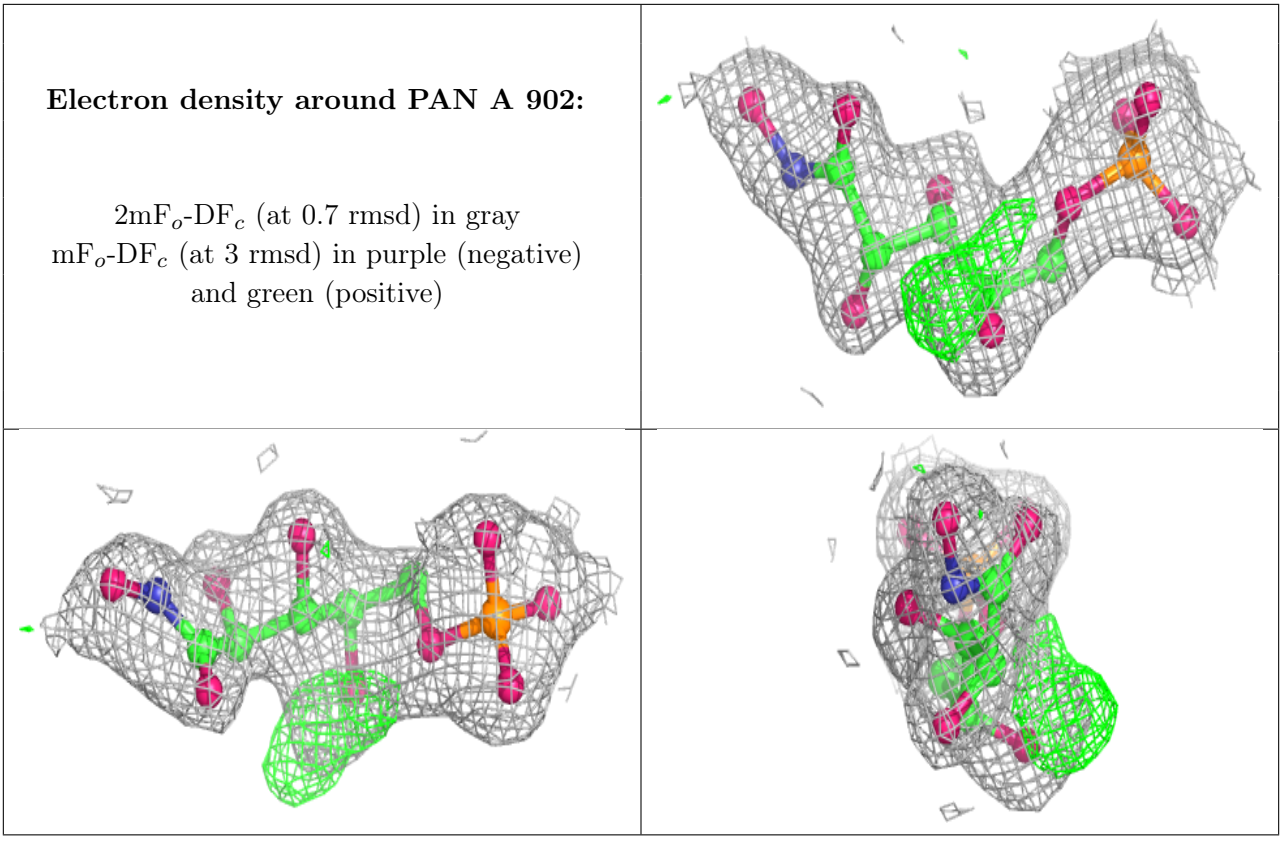
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PAN	A	902	16/16	0.95	0.12	47,50,53,55	0
2	PAN	B	901	16/16	0.95	0.10	30,37,40,41	0

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

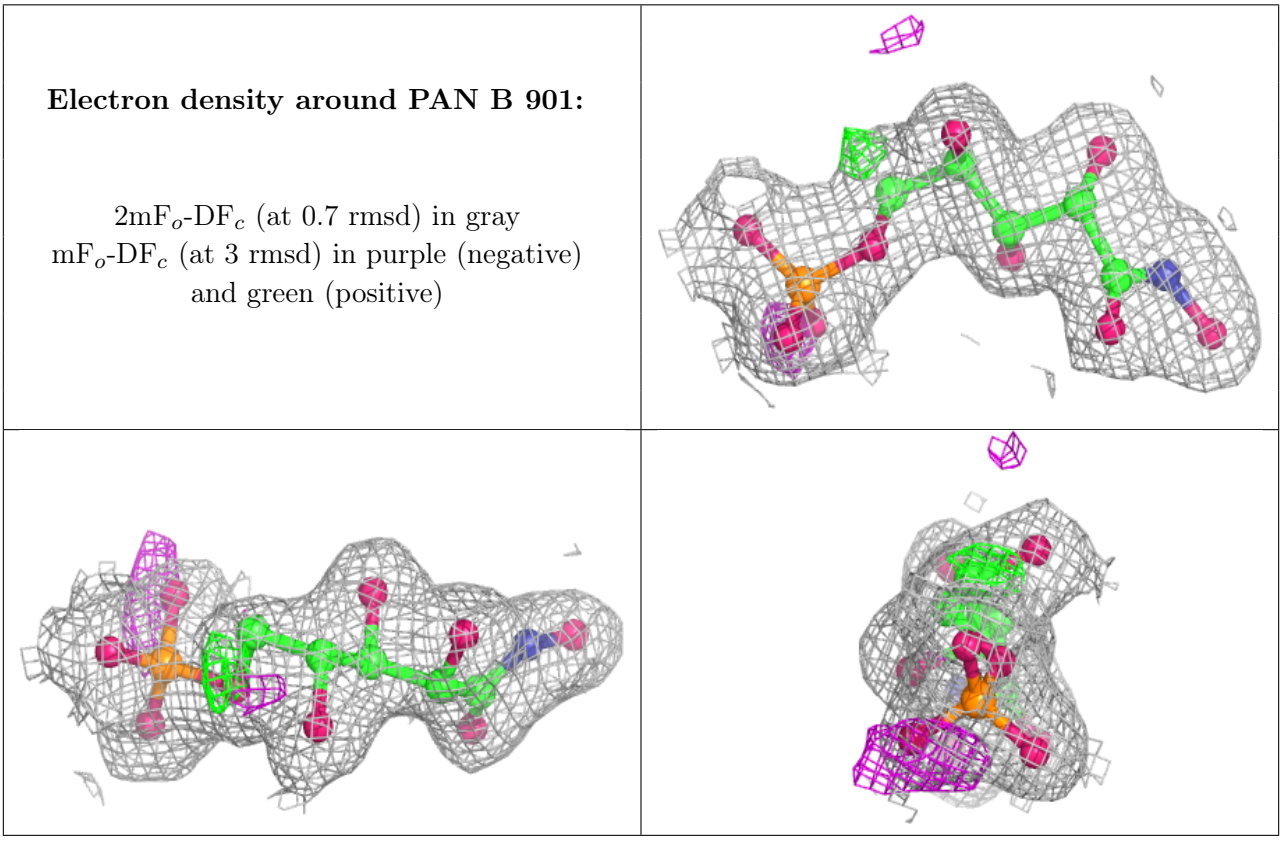
Electron density around PAN A 902:

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



Electron density around PAN B 901:

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



6.5 Other polymers (i)

There are no such residues in this entry.