



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 PM UTC

PDB ID : 6G3U / pdb_00006g3u
Title : Structure of Pseudomonas aeruginosa Isocitrate Dehydrogenase, IDH
Authors : Crousilles, A.; Welch, M.
Deposited on : 2018-03-26
Resolution : 2.71 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

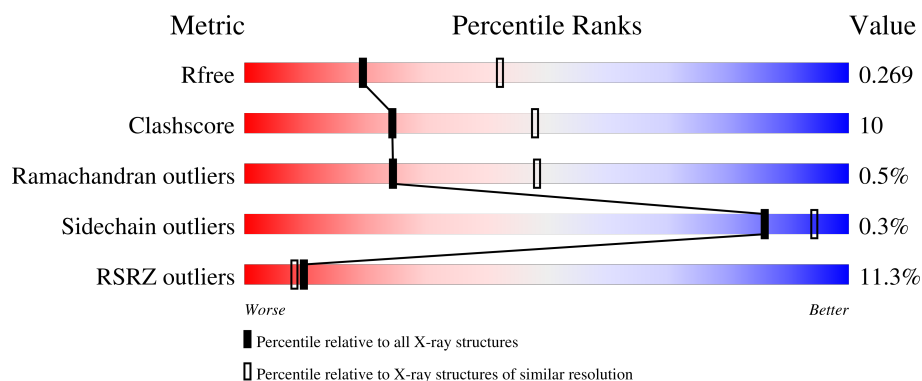
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	737	2% 84% 16%
1	B	737	20% 74% 24%

2 Entry composition [i](#)

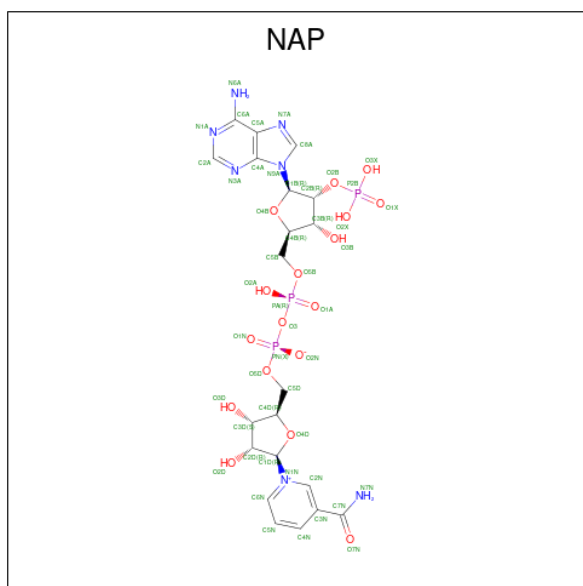
There are 4 unique types of molecules in this entry. The entry contains 11551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

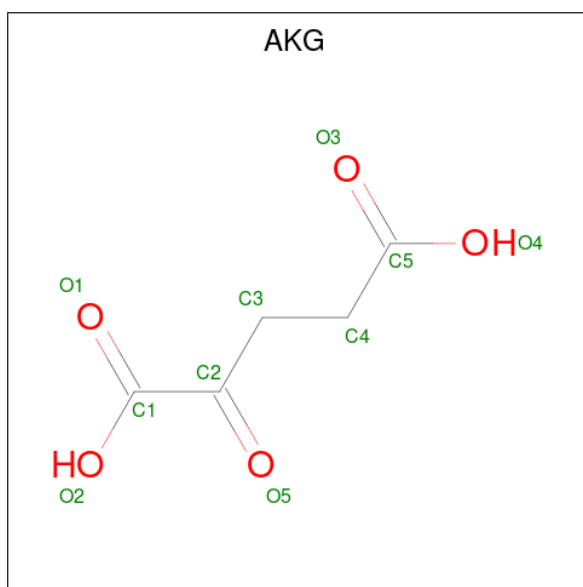
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5695	3584	982	1096	33			
1	B	730	Total	C	N	O	S	0	0	0
			5601	3521	966	1081	33			

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

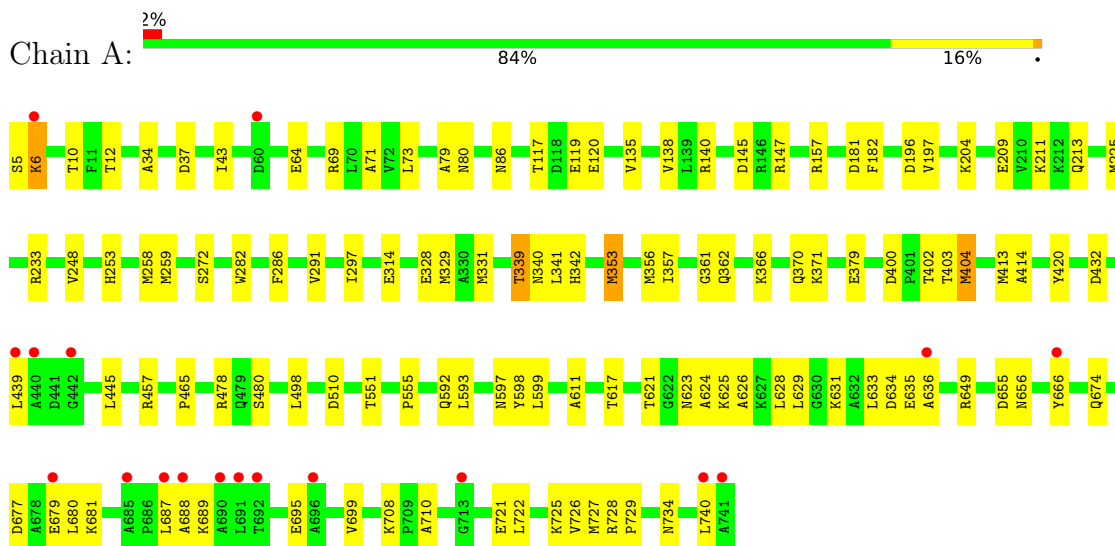
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	78	Total	O	0	0
			78	78		

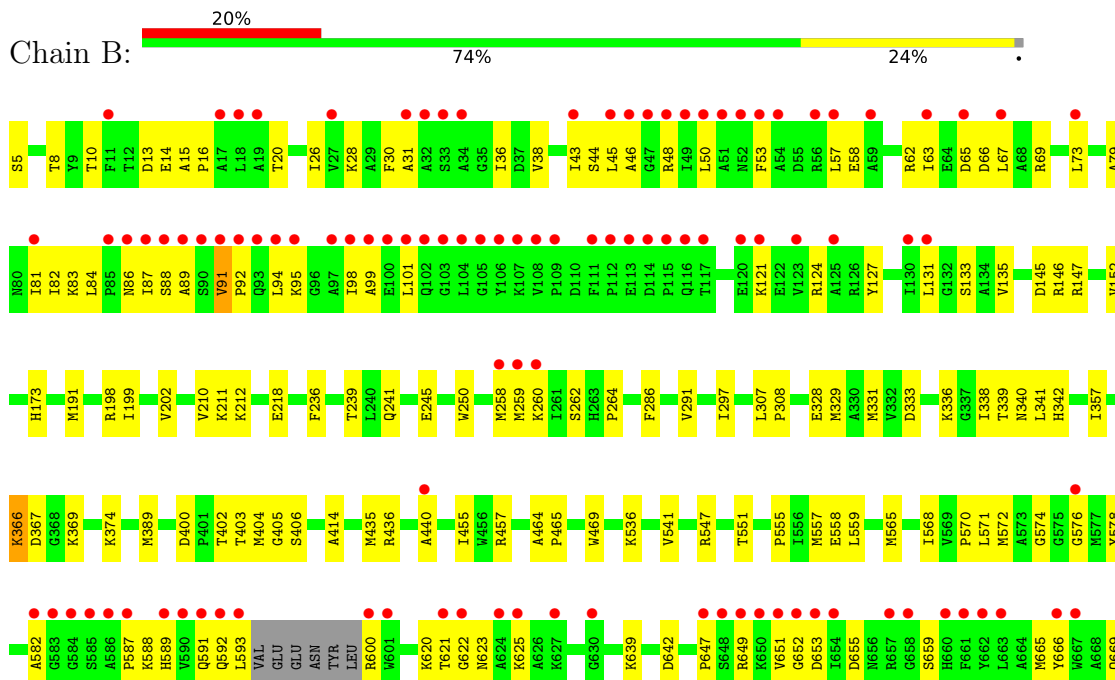
3 Residue-property plots [i](#)

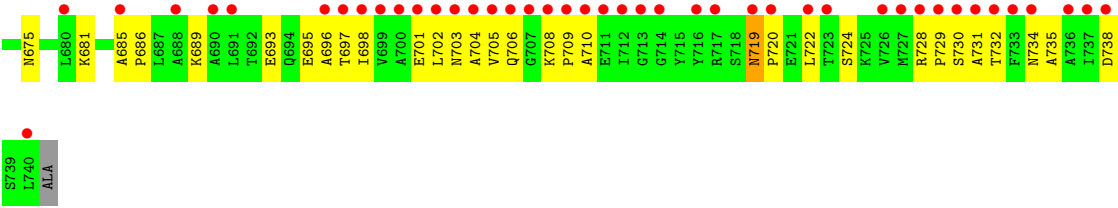
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Isocitrate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.46Å 149.02Å 201.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.71 29.62 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.62-2.71) 99.6 (29.62-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.208 , 0.267 0.210 , 0.269	Depositor DCC
R_{free} test set	2630 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11551	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: NAP, AKG

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	0.46	0/5804	0.71	5/7844 (0.1%)
1	B	0.44	0/5708	0.74	6/7717 (0.1%)
All	All	0.45	0/11512	0.72	11/15561 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	LYS	CB-CG-CD	9.70	133.60	111.30
1	B	258	MET	CB-CG-SD	-8.31	87.77	112.70
1	B	625	LYS	CG-CD-CE	6.40	126.01	111.30
1	A	679	GLU	CB-CG-CD	-5.45	103.34	112.60
1	A	353	MET	CG-SD-CE	-5.33	89.17	100.90
1	B	366	LYS	CD-CE-NZ	-5.17	95.35	111.90
1	B	649	ARG	CA-C-N	5.09	129.56	122.08
1	B	649	ARG	C-N-CA	5.09	129.56	122.08
1	A	404	MET	CB-CG-SD	-5.02	97.65	112.70
1	A	480	SER	CA-C-N	-5.00	115.17	123.37
1	A	480	SER	C-N-CA	-5.00	115.17	123.37

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	5695	0	5673	90	0
1	B	5601	0	5536	133	0
2	A	48	0	25	3	0
3	A	10	0	4	1	0
4	A	119	0	0	2	0
4	B	78	0	0	1	0
All	All	11551	0	11238	223	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 10.

All (223) 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:204:LYS:HE3	1:A:432:ASP:CB	1.85	1.06
1:B:735:ALA:HA	1:B:738:ASP:HB2	1.10	1.05
1:B:328:GLU:HG3	1:B:366:LYS:HE3	1.44	0.99
1:B:731:ALA:HA	1:B:735:ALA:HB3	1.46	0.97
1:A:329:MET:HE1	1:A:341:LEU:HG	1.46	0.95
1:A:204:LYS:HE3	1:A:432:ASP:HB2	1.46	0.94
1:B:94:LEU:HD11	1:B:131:LEU:HD12	1.51	0.93
1:A:636:ALA:HA	1:A:666:TYR:HD2	1.38	0.88
1:A:204:LYS:HE3	1:A:432:ASP:HB3	1.56	0.87
1:A:593:LEU:HD11	1:A:727:MET:HE1	1.58	0.85
1:A:636:ALA:HA	1:A:666:TYR:CD2	2.11	0.84
1:A:329:MET:HE2	1:A:340:ASN:HB3	1.59	0.84
1:A:5:SER:N	1:A:37:ASP:H	1.77	0.82
1:B:14:GLU:HB3	1:B:589:HIS:HB2	1.61	0.81
1:B:236:PHE:O	1:B:239:THR:HG22	1.80	0.81
1:B:91:VAL:HB	1:B:92:PRO:HD3	1.65	0.79
1:A:6:LYS:HE2	1:A:617:THR:HA	1.65	0.78
1:B:239:THR:HG23	1:B:250:TRP:HE1	1.50	0.77
1:B:331:MET:HE1	1:B:339:THR:HG22	1.65	0.76
1:A:331:MET:HE3	1:A:366:LYS:HD2	1.68	0.76
1:A:69:ARG:NH2	4:A:901:HOH:O	2.19	0.76
1:B:621:THR:O	1:B:623:ASN:N	2.21	0.74
1:B:729:PRO:O	1:B:732:THR:OG1	2.02	0.73
1:A:5:SER:O	1:A:6:LYS:HB2	1.87	0.72
1:A:6:LYS:HZ1	1:A:80:ASN:HD22	1.38	0.72
1:B:43:ILE:HD11	1:B:67:LEU:HD13	1.73	0.70
1:B:639:LYS:HD3	1:B:666:TYR:CD1	2.26	0.70
1:B:28:LYS:HD2	1:B:38:VAL:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:MET:HE1	1:B:341:LEU:HG	1.74	0.69
1:B:652:GLY:HA3	1:B:655:ASP:HB2	1.74	0.68
1:A:478:ARG:NH2	1:A:510:ASP:O	2.25	0.68
1:B:50:LEU:HG	1:B:53:PHE:CE2	2.29	0.68
1:B:357:ILE:HG21	1:B:389:MET:HE2	1.74	0.68
1:B:735:ALA:HA	1:B:738:ASP:CB	2.05	0.67
1:A:86:ASN:H	2:A:801:NAP:H71N	1.41	0.67
1:A:621:THR:HG22	1:A:623:ASN:HB2	1.76	0.67
1:B:94:LEU:CD1	1:B:131:LEU:HD12	2.24	0.66
1:B:210:VAL:O	1:B:212:LYS:N	2.27	0.66
1:B:574:GLY:O	1:B:620:LYS:NZ	2.25	0.66
1:B:127:TYR:O	1:B:131:LEU:HD23	1.95	0.65
1:B:730:SER:O	1:B:735:ALA:N	2.17	0.65
1:A:34:ALA:HA	1:A:625:LYS:HD2	1.78	0.64
1:B:58:GLU:HB3	1:B:62:ARG:HH21	1.63	0.64
1:B:587:PRO:O	1:B:588:LYS:HG2	1.98	0.64
1:B:400:ASP:O	1:B:404:MET:HG3	1.97	0.64
1:B:600:ARG:N	1:B:653:ASP:O	2.31	0.63
1:B:46:ALA:O	1:B:50:LEU:N	2.30	0.63
1:A:329:MET:CE	1:A:340:ASN:HB3	2.29	0.63
1:B:703:ASN:HB2	1:B:705:VAL:HG22	1.80	0.63
1:B:53:PHE:HZ	1:B:63:ILE:HG12	1.64	0.63
1:B:14:GLU:HB2	1:B:587:PRO:HB2	1.81	0.62
1:A:253:HIS:CG	1:A:353:MET:HE1	2.34	0.62
1:B:145:ASP:OD2	1:B:147:ARG:NH1	2.32	0.62
1:A:597:ASN:ND2	1:A:710:ALA:HB2	2.15	0.61
1:B:31:ALA:HB1	1:B:36:ILE:CG2	2.29	0.61
1:A:722:LEU:O	1:A:725:LYS:HG3	2.00	0.61
1:B:45:LEU:HD21	1:B:87:ILE:HD11	1.82	0.61
1:B:88:SER:HB3	1:B:133:SER:HB3	1.83	0.61
1:B:735:ALA:CA	1:B:738:ASP:HB2	2.06	0.60
1:A:140:ARG:HH12	3:A:802:AKG:H41	1.66	0.60
1:B:15:ALA:HB3	1:B:587:PRO:O	2.02	0.59
1:B:16:PRO:O	1:B:20:THR:HG23	2.03	0.59
1:B:565:MET:HB2	1:B:582:ALA:CB	2.33	0.59
1:B:357:ILE:HG21	1:B:389:MET:CE	2.32	0.58
1:A:677:ASP:OD1	1:A:680:LEU:N	2.24	0.58
1:B:173:HIS:CE1	1:B:374:LYS:HZ1	2.22	0.58
1:B:14:GLU:HB2	1:B:587:PRO:CB	2.33	0.58
1:B:333:ASP:OD2	1:B:336:LYS:HD2	2.05	0.57
1:B:402:THR:HG22	1:B:403:THR:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LEU:HD22	1:A:445:LEU:HD11	1.85	0.57
1:B:95:LYS:HA	1:B:98:ILE:HG12	1.86	0.57
1:A:10:THR:HG22	1:A:12:THR:HG23	1.87	0.57
1:B:719:ASN:N	1:B:720:PRO:HD3	2.20	0.56
1:A:258:MET:HE2	1:A:420:TYR:CZ	2.41	0.56
1:B:653:ASP:OD2	1:B:709:PRO:HD3	2.05	0.56
1:B:65:ASP:HA	1:B:69:ARG:HD3	1.87	0.56
1:A:282:TRP:HZ2	1:A:314:GLU:HG2	1.70	0.56
1:A:626:ALA:HA	1:A:629:LEU:HD13	1.87	0.56
1:A:253:HIS:CB	1:A:353:MET:HE1	2.35	0.56
1:B:367:ASP:OD2	1:B:369:LYS:HD2	2.07	0.56
1:A:140:ARG:HD3	1:A:413:MET:SD	2.46	0.55
1:A:400:ASP:O	1:A:404:MET:HB2	2.05	0.55
1:B:400:ASP:OD1	1:B:402:THR:HB	2.07	0.54
1:B:26:ILE:HD11	1:B:30:PHE:CE1	2.41	0.54
1:A:635:GLU:C	1:A:666:TYR:HE2	2.15	0.54
1:B:86:ASN:HD21	1:B:135:VAL:HG21	1.72	0.54
1:B:639:LYS:HA	1:B:642:ASP:HB2	1.90	0.54
1:B:406:SER:OG	1:B:558:GLU:OE2	2.20	0.53
1:A:181:ASP:HB2	1:A:379:GLU:OE1	2.08	0.53
1:A:86:ASN:O	2:A:801:NAP:H2N	2.08	0.53
1:B:389:MET:CE	1:B:557:MET:HE3	2.39	0.53
1:B:414:ALA:HB3	1:B:465:PRO:HB3	1.90	0.52
1:B:389:MET:HE1	1:B:557:MET:HE3	1.91	0.52
1:A:727:MET:C	1:A:729:PRO:HD3	2.34	0.52
1:A:728:ARG:O	1:A:734:ASN:ND2	2.35	0.52
1:B:241:GLN:NE2	1:B:245:GLU:OE1	2.43	0.52
1:A:339:THR:HG23	1:A:341:LEU:H	1.75	0.52
1:B:675:ASN:HD21	1:B:681:LYS:NZ	2.08	0.52
1:B:5:SER:OG	1:B:36:ILE:HD12	2.10	0.51
1:B:259:MET:HE2	1:B:457:ARG:HH11	1.74	0.51
1:B:152:VAL:HG12	1:B:559:LEU:HD22	1.92	0.51
1:B:145:ASP:OD1	1:B:147:ARG:HD3	2.10	0.51
1:B:731:ALA:CA	1:B:735:ALA:HB3	2.30	0.51
1:A:674:GLN:O	1:A:681:LYS:HD2	2.11	0.51
1:B:665:MET:HE3	1:B:669:GLN:OE1	2.10	0.51
1:A:726:VAL:HG12	1:A:727:MET:HE2	1.93	0.51
1:A:297:ILE:HG22	1:A:342:HIS:HA	1.93	0.50
1:B:10:THR:HG23	1:B:82:ILE:O	2.11	0.50
1:B:50:LEU:HD13	1:B:66:ASP:HB3	1.94	0.50
1:A:624:ALA:O	1:A:628:LEU:HD22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:LEU:HD11	1:A:727:MET:CE	2.38	0.50
1:B:199:ILE:O	1:B:210:VAL:O	2.29	0.50
1:A:649:ARG:NH1	2:A:801:NAP:O2X	2.45	0.49
1:B:173:HIS:CE1	1:B:374:LYS:NZ	2.80	0.49
1:A:209:GLU:OE1	1:A:211:LYS:NZ	2.44	0.49
1:B:297:ILE:HG22	1:B:342:HIS:HA	1.95	0.49
1:A:145:ASP:OD2	1:A:147:ARG:NH1	2.46	0.49
1:A:328:GLU:OE2	1:A:371:LYS:NZ	2.35	0.49
1:B:706:GLN:HB3	1:B:710:ALA:HB3	1.94	0.49
1:A:611:ALA:HB2	1:A:633:LEU:HD23	1.95	0.49
1:B:202:VAL:HG21	1:B:436:ARG:NH1	2.27	0.49
1:B:260:LYS:O	1:B:264:PRO:HG2	2.13	0.49
1:B:333:ASP:HB3	1:B:338:ILE:HD12	1.95	0.48
1:B:50:LEU:C	1:B:50:LEU:HD23	2.39	0.48
1:A:6:LYS:O	1:A:80:ASN:HB3	2.13	0.48
1:A:43:ILE:HD12	1:A:135:VAL:HG11	1.96	0.48
1:B:173:HIS:NE2	1:B:374:LYS:NZ	2.62	0.48
1:B:724:SER:OG	1:B:728:ARG:HD3	2.14	0.48
1:A:5:SER:O	1:A:5:SER:OG	2.29	0.48
1:B:50:LEU:HD13	1:B:66:ASP:CB	2.44	0.47
1:A:370:GLN:C	1:A:371:LYS:HG3	2.39	0.47
1:A:625:LYS:HA	1:A:628:LEU:HD23	1.96	0.47
1:B:329:MET:HE3	1:B:340:ASN:HB3	1.95	0.47
1:B:695:GLU:HG3	1:B:696:ALA:N	2.29	0.47
1:B:83:LYS:HD2	1:B:83:LYS:C	2.40	0.47
1:A:725:LYS:HE3	1:A:726:VAL:HG23	1.96	0.47
1:B:16:PRO:HD2	1:B:587:PRO:HB3	1.97	0.47
1:B:239:THR:CG2	1:B:250:TRP:HE1	2.22	0.47
1:A:402:THR:HG22	1:A:403:THR:HG23	1.97	0.47
1:B:53:PHE:CZ	1:B:63:ILE:HG12	2.47	0.47
1:B:198:ARG:NH2	1:B:440:ALA:HA	2.30	0.47
1:A:64:GLU:OE1	1:A:69:ARG:HD3	2.15	0.46
1:A:598:TYR:CE1	1:A:655:ASP:HB3	2.50	0.46
1:A:599:LEU:HD23	1:A:656:ASN:HB3	1.96	0.46
1:B:83:LYS:HD2	1:B:84:LEU:O	2.16	0.46
1:B:720:PRO:HB2	1:B:722:LEU:HG	1.97	0.46
1:B:43:ILE:CD1	1:B:67:LEU:HD13	2.44	0.46
1:B:329:MET:HE2	1:B:339:THR:HB	1.98	0.46
1:B:647:PRO:HD3	1:B:659:SER:OG	2.16	0.46
1:A:414:ALA:HB3	1:A:465:PRO:HB3	1.98	0.46
1:B:697:THR:O	1:B:701:GLU:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:NZ	1:A:80:ASN:HD22	2.11	0.46
1:A:687:LEU:HD22	1:A:740:LEU:HD12	1.98	0.46
1:B:13:ASP:OD1	1:B:44:SER:HB2	2.16	0.46
1:A:721:GLU:CD	1:A:721:GLU:H	2.24	0.45
1:B:14:GLU:CB	1:B:587:PRO:HB2	2.46	0.45
1:B:703:ASN:C	1:B:705:VAL:H	2.24	0.45
1:A:119:GLU:OE1	1:A:119:GLU:N	2.44	0.45
1:A:353:MET:HB2	1:A:353:MET:HE2	1.32	0.45
1:A:196:ASP:OD2	1:A:213:GLN:NE2	2.42	0.45
1:A:356:MET:HE2	1:A:357:ILE:HG13	1.98	0.45
1:A:439:LEU:HD12	1:A:439:LEU:HA	1.69	0.45
1:A:117:THR:HG23	1:A:120:GLU:OE1	2.17	0.44
1:B:329:MET:CE	1:B:340:ASN:HB3	2.48	0.44
1:A:592:GLN:HG2	1:A:598:TYR:O	2.17	0.44
1:B:89:ALA:HB2	1:B:133:SER:N	2.32	0.44
1:B:239:THR:HG23	1:B:250:TRP:NE1	2.28	0.44
1:B:262:SER:HB3	1:B:455:ILE:HG21	1.99	0.44
1:B:551:THR:O	1:B:555:PRO:HG2	2.18	0.44
1:B:675:ASN:HD21	1:B:681:LYS:HZ3	1.64	0.44
1:A:73:LEU:O	1:A:79:ALA:HB2	2.18	0.44
1:A:362:GLN:OE1	1:A:370:GLN:HG3	2.17	0.44
1:B:92:PRO:O	1:B:95:LYS:HB2	2.18	0.44
1:A:233:ARG:HH12	1:A:272:SER:HB2	1.83	0.43
1:B:639:LYS:HD3	1:B:666:TYR:CE1	2.52	0.43
1:A:282:TRP:CZ2	1:A:314:GLU:HG2	2.52	0.43
1:B:286:PHE:O	1:B:291:VAL:HG12	2.18	0.43
1:B:571:LEU:HD12	1:B:576:GLY:N	2.34	0.43
1:B:591:GLN:NE2	4:B:808:HOH:O	2.45	0.43
1:B:73:LEU:O	1:B:79:ALA:HB2	2.19	0.43
1:B:98:ILE:HG13	1:B:99:ALA:N	2.34	0.43
1:B:464:ALA:HB3	1:B:465:PRO:HD3	2.00	0.43
1:A:498:LEU:HD12	1:A:498:LEU:HA	1.69	0.43
1:B:728:ARG:C	1:B:730:SER:N	2.77	0.43
1:B:83:LYS:HD2	1:B:84:LEU:N	2.35	0.42
1:B:307:LEU:HB3	1:B:308:PRO:HD2	2.01	0.42
1:A:286:PHE:HB3	1:A:291:VAL:HG22	2.02	0.42
1:B:146:ARG:HH12	1:B:547:ARG:HH11	1.67	0.42
1:B:702:LEU:O	1:B:704:ALA:N	2.52	0.42
1:A:625:LYS:HB3	1:A:625:LYS:HE2	1.84	0.42
1:B:435:MET:HE3	1:B:435:MET:HB3	1.89	0.42
1:B:685:ALA:N	1:B:686:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:ASN:O	1:B:738:ASP:N	2.47	0.42
1:A:457:ARG:NH2	4:A:909:HOH:O	2.52	0.42
1:B:121:LYS:O	1:B:124:ARG:HB3	2.20	0.42
1:B:592:GLN:CD	1:B:593:LEU:H	2.27	0.42
1:B:647:PRO:HB3	1:B:651:VAL:O	2.20	0.42
1:A:157:ARG:HD3	1:A:402:THR:O	2.20	0.41
1:A:688:ALA:HB3	1:A:689:LYS:HD2	2.01	0.41
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.78	0.41
1:B:191:MET:HB2	1:B:218:GLU:O	2.20	0.41
1:B:469:TRP:CZ2	1:B:541:VAL:HG12	2.55	0.41
1:B:565:MET:HB2	1:B:582:ALA:HB3	2.02	0.41
1:B:89:ALA:HB2	1:B:133:SER:H	1.86	0.41
1:B:464:ALA:HB1	1:B:572:MET:HE1	2.02	0.41
1:B:708:LYS:N	1:B:709:PRO:HD2	2.36	0.41
1:A:71:ALA:HB2	1:A:138:VAL:CG1	2.51	0.41
1:A:631:LYS:HD3	1:A:634:ASP:HB2	2.02	0.41
1:B:568:ILE:HG22	1:B:570:PRO:HD3	2.03	0.41
1:A:286:PHE:HB3	1:A:291:VAL:CG2	2.51	0.41
1:B:728:ARG:C	1:B:730:SER:H	2.29	0.41
1:A:551:THR:O	1:A:555:PRO:HG2	2.21	0.40
1:A:597:ASN:HB2	1:A:708:LYS:O	2.22	0.40
1:A:204:LYS:CE	1:A:432:ASP:HB2	2.31	0.40
1:A:259:MET:HE3	1:A:259:MET:HB3	1.97	0.40
1:B:48:ARG:NH2	1:B:101:LEU:HD13	2.35	0.40
1:B:405:GLY:HA3	1:B:536:LYS:O	2.21	0.40
1:A:356:MET:HE3	1:A:361:GLY:HA2	2.03	0.40
1:B:87:ILE:O	1:B:87:ILE:HG13	2.21	0.40
1:A:182:PHE:CD1	1:A:225:MET:HG3	2.56	0.40
1:A:695:GLU:O	1:A:699:VAL:HG23	2.22	0.40
1:B:8:THR:O	1:B:81:ILE:HA	2.22	0.40
1:B:689:LYS:O	1:B:693:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	735/737 (100%)	704 (96%)	30 (4%)	1 (0%)	48	73
1	B	726/737 (98%)	668 (92%)	51 (7%)	7 (1%)	12	32
All	All	1461/1474 (99%)	1372 (94%)	81 (6%)	8 (0%)	24	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	B	57	LEU
1	B	211	LYS
1	B	578	TYR
1	B	622	GLY
1	B	91	VAL
1	B	698	ILE
1	B	719	ASN

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	607/607 (100%)	604 (100%)	3 (0%)	81	92
1	B	592/607 (98%)	592 (100%)	0	100	100
All	All	1199/1214 (99%)	1196 (100%)	3 (0%)	86	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	VAL
1	A	248	VAL
1	A	339	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	159	HIS
1	A	241	GLN
1	A	396	ASN
1	A	683	HIS
1	B	86	ASN
1	B	213	GLN
1	B	241	GLN
1	B	359	ASN
1	B	362	GLN
1	B	370	GLN
1	B	396	ASN
1	B	409	ASN
1	B	660	HIS
1	B	675	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	801	-	50,52,52	1.49	5 (10%)	71,80,80	1.67	15 (21%)
3	AKG	A	802	-	9,9,9	1.59	3 (33%)	11,11,11	2.46	4 (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	NAP	A	801	-	-	13/35/67/67	0/5/5/5
3	AKG	A	802	-	-	4/9/9/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	O7N-C7N	7.89	1.38	1.24
2	A	801	NAP	C2A-N3A	2.53	1.38	1.33
2	A	801	NAP	C2A-N1A	2.37	1.38	1.33
3	A	802	AKG	C2-C1	-2.34	1.50	1.53
2	A	801	NAP	C8A-N7A	2.29	1.36	1.31
3	A	802	AKG	O5-C2	-2.21	1.18	1.23
2	A	801	NAP	C2N-N1N	2.05	1.37	1.35
3	A	802	AKG	O2-C1	-2.05	1.25	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAP	N3A-C2A-N1A	-5.73	119.90	128.58
3	A	802	AKG	C3-C4-C5	-4.68	101.26	113.67
3	A	802	AKG	C4-C3-C2	-4.64	104.21	112.91
2	A	801	NAP	N9A-C8A-N7A	-3.76	108.60	113.94
2	A	801	NAP	C2B-C1B-N9A	-3.55	107.91	113.75
3	A	802	AKG	C3-C2-C1	3.46	121.73	115.86
2	A	801	NAP	C5A-C4A-N3A	-3.37	122.07	126.72
2	A	801	NAP	C5N-C4N-C3N	-3.25	117.17	120.36
2	A	801	NAP	C6N-N1N-C2N	-3.18	119.17	121.88
2	A	801	NAP	C2A-N3A-C4A	2.97	119.07	111.83
2	A	801	NAP	C5A-N7A-C8A	2.95	108.09	103.45
2	A	801	NAP	O2B-P2B-O1X	-2.24	101.34	109.33
2	A	801	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
2	A	801	NAP	O2N-PN-O1N	2.16	122.51	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	AKG	O4-C5-C4	2.14	120.77	114.00
2	A	801	NAP	C4A-N9A-C8A	2.13	107.97	105.74
2	A	801	NAP	O2B-C2B-C1B	-2.11	102.64	110.05
2	A	801	NAP	O7N-C7N-N7N	-2.04	119.67	122.62
2	A	801	NAP	N3A-C4A-N9A	2.03	130.63	127.17

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C5B-O5B-PA-O1A
2	A	801	NAP	C5B-O5B-PA-O2A
2	A	801	NAP	C5B-O5B-PA-O3
2	A	801	NAP	C5D-O5D-PN-O3
2	A	801	NAP	C5D-O5D-PN-O1N
2	A	801	NAP	O4D-C1D-N1N-C2N
2	A	801	NAP	O4D-C1D-N1N-C6N
3	A	802	AKG	O2-C1-C2-C3
2	A	801	NAP	O4B-C4B-C5B-O5B
2	A	801	NAP	C3B-C4B-C5B-O5B
2	A	801	NAP	PA-O3-PN-O5D
3	A	802	AKG	O1-C1-C2-O5
3	A	802	AKG	O1-C1-C2-C3
2	A	801	NAP	C5D-O5D-PN-O2N
3	A	802	AKG	C2-C3-C4-C5
2	A	801	NAP	C2D-C1D-N1N-C2N
2	A	801	NAP	PA-O3-PN-O2N

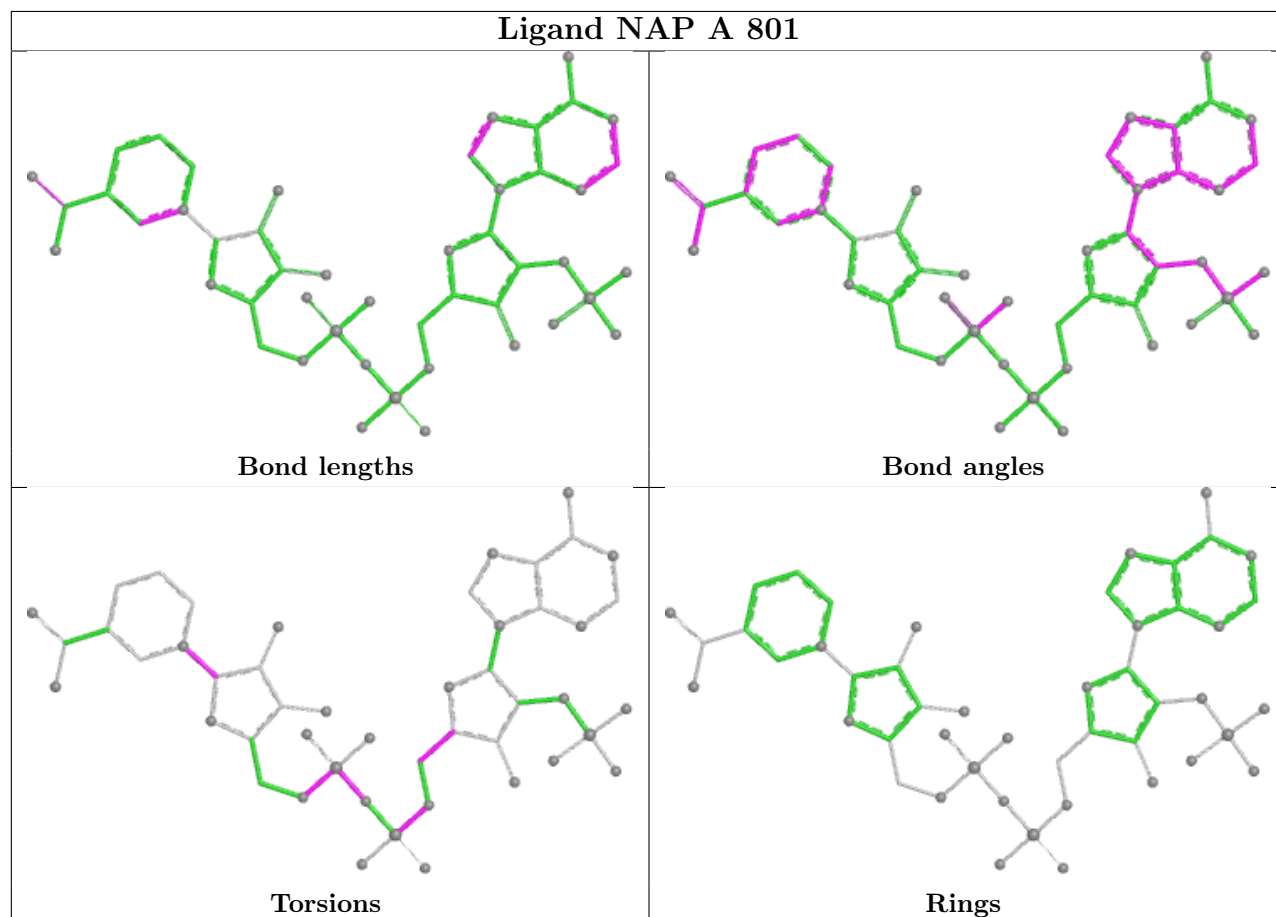
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAP	3	0
3	A	802	AKG	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	737/737 (100%)	-0.11	18 (2%) 59 56	19, 38, 71, 88	0
1	B	730/737 (99%)	0.75	148 (20%) 3 2	19, 51, 135, 159	0
All	All	1467/1474 (99%)	0.32	166 (11%) 10 8	19, 43, 120, 159	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LEU	6.4
1	B	108	VAL	6.3
1	B	91	VAL	5.3
1	B	731	ALA	5.2
1	B	109	PRO	5.2
1	B	104	LEU	4.9
1	B	585	SER	4.9
1	B	592	GLN	4.9
1	B	593	LEU	4.9
1	B	94	LEU	4.9
1	B	654	ILE	4.9
1	B	700	ALA	4.5
1	B	710	ALA	4.5
1	B	733	PHE	4.5
1	B	714	GLY	4.4
1	B	115	PRO	4.4
1	B	18	LEU	4.3
1	B	701	GLU	4.2
1	B	89	ALA	4.2
1	B	106	TYR	4.2
1	B	707	GLY	4.2
1	B	48	ARG	4.1
1	B	17	ALA	4.1
1	B	586	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	583	GLY	4.1
1	B	740	LEU	4.1
1	B	651	VAL	4.1
1	B	54	ALA	4.0
1	B	19	ALA	4.0
1	B	589	HIS	4.0
1	B	738	ASP	4.0
1	B	576	GLY	3.9
1	B	590	VAL	3.9
1	B	712	ILE	3.8
1	B	90	SER	3.8
1	B	98	ILE	3.8
1	B	582	ALA	3.8
1	B	647	PRO	3.7
1	B	727	MET	3.7
1	B	92	PRO	3.7
1	B	702	LEU	3.7
1	A	666	TYR	3.7
1	B	726	VAL	3.7
1	B	27	VAL	3.6
1	B	45	LEU	3.6
1	B	699	VAL	3.6
1	B	59	ALA	3.6
1	B	103	GLY	3.6
1	B	258	MET	3.5
1	B	105	GLY	3.5
1	B	601	TRP	3.5
1	B	732	THR	3.5
1	B	51	ALA	3.5
1	B	696	ALA	3.5
1	B	259	MET	3.5
1	B	713	GLY	3.5
1	B	50	LEU	3.5
1	B	47	GLY	3.5
1	B	703	ASN	3.4
1	B	666	TYR	3.4
1	B	87	ILE	3.4
1	B	57	LEU	3.4
1	B	102	GLN	3.3
1	B	625	LYS	3.3
1	B	112	PRO	3.3
1	B	704	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	49	ILE	3.3
1	B	123	VAL	3.3
1	B	97	ALA	3.2
1	B	600	ARG	3.2
1	B	698	ILE	3.2
1	B	653	ASP	3.2
1	B	691	LEU	3.2
1	B	65	ASP	3.1
1	A	741	ALA	3.1
1	B	657	ARG	3.1
1	B	31	ALA	3.0
1	B	706	GLN	3.0
1	B	440	ALA	3.0
1	B	63	ILE	3.0
1	B	630	GLY	2.9
1	B	652	GLY	2.9
1	B	667	TRP	2.9
1	B	260	LYS	2.9
1	B	93	GLN	2.8
1	B	99	ALA	2.8
1	B	587	PRO	2.8
1	B	32	ALA	2.8
1	B	708	LYS	2.8
1	B	622	GLY	2.8
1	B	53	PHE	2.8
1	B	120	GLU	2.8
1	B	95	LYS	2.7
1	B	661	PHE	2.7
1	B	43	ILE	2.7
1	B	584	GLY	2.7
1	B	730	SER	2.7
1	B	34	ALA	2.7
1	B	125	ALA	2.7
1	B	111	PHE	2.7
1	B	734	ASN	2.7
1	B	705	VAL	2.7
1	B	113	GLU	2.6
1	B	737	ILE	2.6
1	A	439	LEU	2.6
1	B	107	LYS	2.6
1	B	688	ALA	2.6
1	B	722	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	729	PRO	2.5
1	B	116	GLN	2.5
1	B	685	ALA	2.5
1	B	736	ALA	2.5
1	A	691	LEU	2.5
1	B	67	LEU	2.5
1	A	440	ALA	2.4
1	A	685	ALA	2.4
1	B	697	THR	2.4
1	B	680	LEU	2.4
1	B	33	SER	2.4
1	B	690	ALA	2.4
1	A	60	ASP	2.4
1	B	114	ASP	2.4
1	B	658	GLY	2.4
1	B	100	GLU	2.3
1	B	709	PRO	2.3
1	B	11	PHE	2.3
1	B	130	ILE	2.3
1	B	88	SER	2.3
1	B	56	ARG	2.3
1	A	442	GLY	2.3
1	B	85	PRO	2.2
1	B	81	ILE	2.2
1	B	650	LYS	2.2
1	B	716	TYR	2.2
1	B	131	LEU	2.2
1	B	711	GLU	2.2
1	B	648	SER	2.2
1	B	663	LEU	2.2
1	B	621	THR	2.2
1	B	649	ARG	2.2
1	B	717	ARG	2.2
1	B	728	ARG	2.2
1	B	86	ASN	2.2
1	A	6	LYS	2.2
1	A	740	LEU	2.2
1	B	73	LEU	2.2
1	A	688	ALA	2.1
1	B	723	THR	2.1
1	B	719	ASN	2.1
1	A	687	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	713	GLY	2.1
1	B	121	LYS	2.1
1	B	660	HIS	2.1
1	B	662	TYR	2.1
1	A	636	ALA	2.1
1	A	679	GLU	2.1
1	A	690	ALA	2.1
1	B	46	ALA	2.1
1	B	117	THR	2.1
1	B	720	PRO	2.1
1	B	624	ALA	2.0
1	B	591	GLN	2.0
1	A	696	ALA	2.0
1	B	627	LYS	2.0
1	A	692	THR	2.0
1	B	52	ASN	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](#)

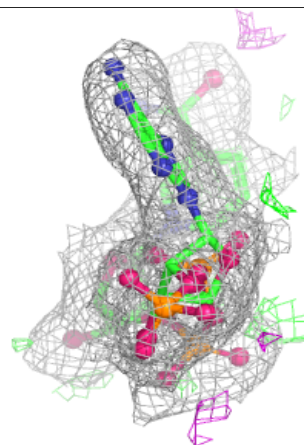
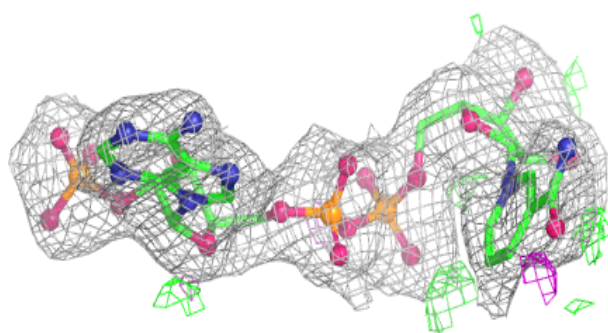
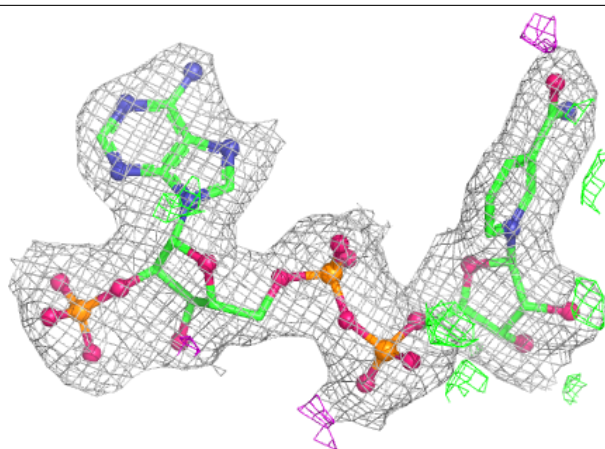
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AKG	A	802	10/10	0.87	0.16	25,33,41,44	0
2	NAP	A	801	48/48	0.98	0.05	19,27,36,41	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 NAP A 801:

$2mF_o-DF_c$ (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.