



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 12:05 PM BST

PDB ID : 3VHM
Title : Crystal structure of NPC-biotin-avidin complex
Authors : Terai, T.; Maki, E.; Sugiyama, S.; Takahashi, Y.; Matsumura, H.; Mori, Y.; Nagano, T.
Deposited on : 2011-08-29
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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

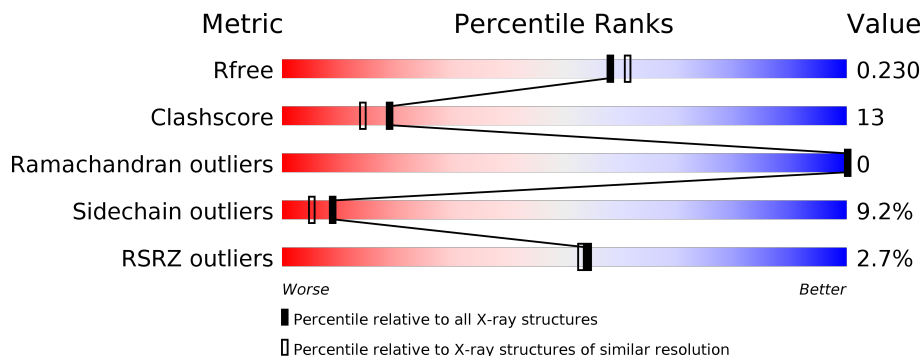
1 Overall quality at a glance

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}	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)
RSRZ outliers	127900	7900 (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 on 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	123	 3% 78% 18% •
1	B	123	 3% 76% 17% 5% •
1	C	123	 3% 75% 20% 5% •
1	D	123	 3% 76% 17% 6% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	1127	-	-	X	-
4	SO4	D	1126	-	-	X	-

2 Entry composition [i](#)

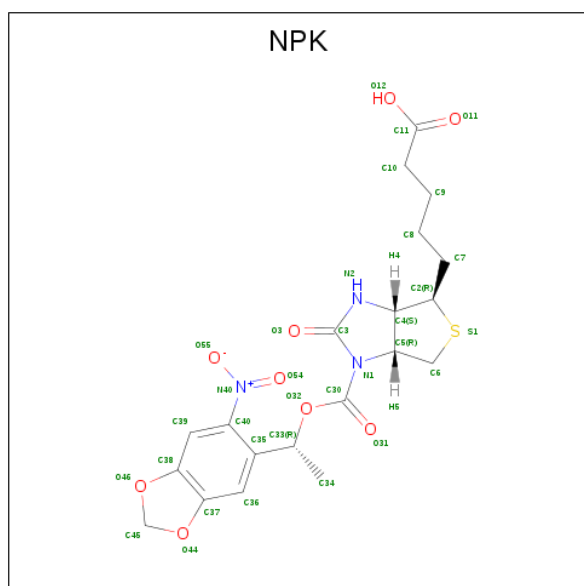
There are 5 unique types of molecules in this entry. The entry contains 4241 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Avidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	123	Total 964	C 603	N 171	O 186	S 4	0	0	0
1	B	121	Total 948	C 594	N 166	O 184	S 4	0	0	0
1	C	123	Total 961	C 602	N 170	O 185	S 4	0	0	0
1	D	121	Total 948	C 594	N 166	O 184	S 4	0	0	0

- Molecule 2 is 5-[(3aS,4R,6aR)-1-[[[(1R)-1-(6-nitro-1,3-benzodioxol-5-yl)ethoxy]carbonyl]-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]pentanoic acid (three-letter code: NPK) (formula: C₂₀H₂₃N₃O₉S).



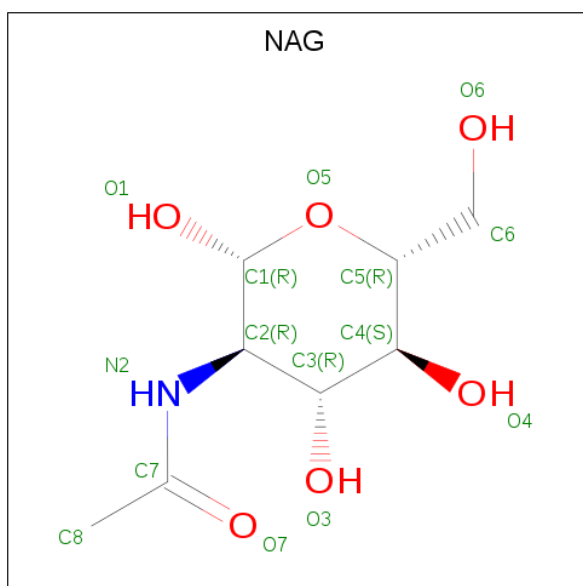
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 33	C 20	N 3	O 9	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	Total 33	C 20	N 3	O 9	S 1	0	0
2	C	1	Total 33	C 20	N 3	O 9	S 1	0	0
2	D	1	Total 33	C 20	N 3	O 9	S 1	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	C	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	D	1	5	4	1	0	0

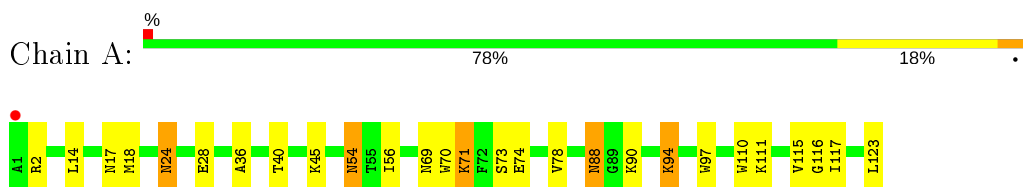
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	51	51	51	0	0
5	B	45	45	45	0	0
5	C	57	57	57	0	0
5	D	49	49	49	0	0

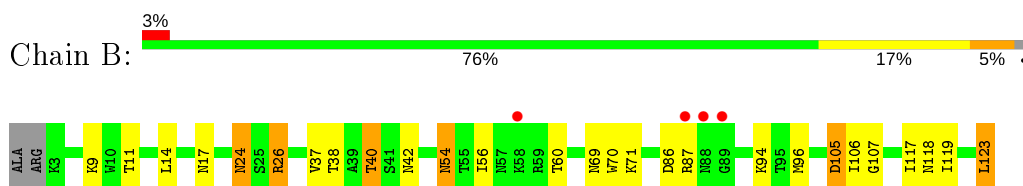
3 Residue-property plots [i](#)

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.

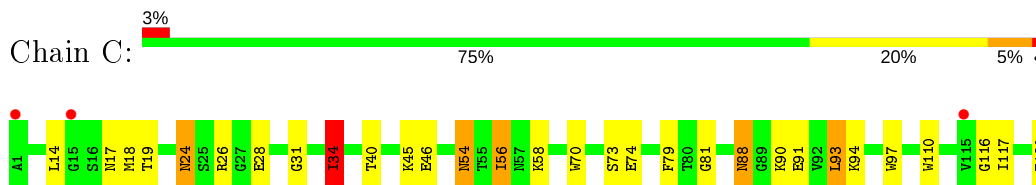
- Molecule 1: Avidin



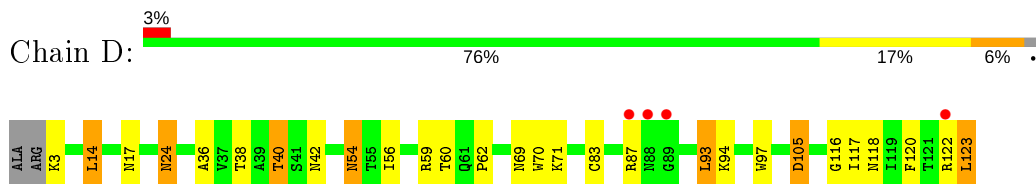
- Molecule 1: Avidin



- Molecule 1: Avidin



- Molecule 1: Avidin



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.02Å 73.53Å 81.18Å 90.00° 120.02° 90.00°	Depositor
Resolution (Å)	37.52 – 2.00 37.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.52-2.00) 98.2 (37.52-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.230 0.190 , 0.230	Depositor DCC
R_{free} test set	2228 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.003 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.009 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4241	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NPK, SO4

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	1.34	5/982 (0.5%)	1.09	2/1328 (0.2%)
1	B	1.28	0/966	1.06	1/1307 (0.1%)
1	C	1.31	1/979 (0.1%)	1.05	1/1324 (0.1%)
1	D	1.35	0/966	1.09	2/1307 (0.2%)
All	All	1.32	6/3893 (0.2%)	1.07	6/5266 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	TRP	CB-CG	5.90	1.60	1.50
1	A	115	VAL	CB-CG1	5.59	1.64	1.52
1	C	79	PHE	CD1-CE1	5.40	1.50	1.39
1	A	74	GLU	CB-CG	5.39	1.62	1.52
1	A	78	VAL	CB-CG1	5.18	1.63	1.52
1	A	110	TRP	CZ3-CH2	5.08	1.48	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	2	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	34	ILE	CB-CA-C	-5.53	100.54	111.60
1	A	2	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	26	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	123	LEU	CA-CB-CG	5.25	127.37	115.30

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	964	0	953	25	0
1	B	948	0	933	28	0
1	C	961	0	950	30	0
1	D	948	0	933	25	0
2	A	33	0	19	6	0
2	B	33	0	19	4	0
2	C	33	0	21	4	0
2	D	33	0	19	3	0
3	A	14	0	13	2	0
3	B	14	0	13	2	0
3	C	14	0	13	6	0
3	D	14	0	13	5	0
4	A	10	0	0	0	0
4	B	10	0	0	2	0
4	C	5	0	0	0	0
4	D	5	0	0	3	0
5	A	51	0	0	0	0
5	B	45	0	0	0	0
5	C	57	0	0	0	0
5	D	49	0	0	0	0
All	All	4241	0	3899	99	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 13.

All (99) 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:B:17:ASN:HD21	3:B:1125:NAG:C1	1.00	1.61
1:C:17:ASN:HD21	3:C:1125:NAG:C1	1.11	1.60
1:D:17:ASN:HD21	3:D:1125:NAG:C1	0.91	1.54
1:C:17:ASN:HD21	3:C:1125:NAG:C2	1.58	1.16
1:D:40:THR:HG23	1:D:42:ASN:H	1.27	0.97
1:B:40:THR:HG23	1:B:42:ASN:H	1.27	0.96
1:C:17:ASN:CG	3:C:1125:NAG:C1	2.44	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TRP:CZ2	2:A:1124:NPK:H8A	2.11	0.85
1:B:60:THR:HG23	4:B:1127:SO4:O2	1.78	0.82
1:C:74:GLU:CD	1:D:59:ARG:HD2	2.01	0.79
1:D:40:THR:HG23	1:D:42:ASN:N	2.00	0.76
1:C:14:LEU:HD13	2:C:1124:NPK:H45	1.66	0.76
1:D:17:ASN:HD21	3:D:1125:NAG:C2	1.94	0.75
1:B:40:THR:HG23	1:B:42:ASN:N	2.02	0.75
1:A:24:ASN:HD22	1:A:24:ASN:C	1.92	0.73
1:B:9:LYS:HE2	1:B:123:LEU:HD13	1.71	0.72
1:A:17:ASN:ND2	3:A:1125:NAG:C2	2.51	0.72
1:A:17:ASN:CG	3:A:1125:NAG:C1	2.57	0.70
1:D:118:ASN:HA	2:D:1124:NPK:O54	1.91	0.70
1:B:24:ASN:HD22	1:B:24:ASN:C	1.95	0.70
1:D:17:ASN:CG	3:D:1125:NAG:C1	2.62	0.67
1:C:17:ASN:OD1	3:C:1125:NAG:C1	2.44	0.66
1:C:70:TRP:CZ2	2:C:1124:NPK:H8A	2.32	0.64
1:C:24:ASN:C	1:C:24:ASN:HD22	1.99	0.64
1:C:74:GLU:OE1	1:D:59:ARG:HD2	1.97	0.64
1:C:91:GLU:OE1	1:C:122:ARG:NH1	2.31	0.64
1:D:60:THR:HG23	4:D:1126:SO4:O4	1.97	0.63
1:D:17:ASN:ND2	3:D:1125:NAG:C2	2.56	0.63
1:B:70:TRP:CZ2	2:B:1124:NPK:H8A	2.34	0.63
1:B:118:ASN:HA	2:B:1124:NPK:O54	1.99	0.63
1:C:17:ASN:ND2	3:C:1125:NAG:C2	2.39	0.63
1:B:9:LYS:HE2	1:B:123:LEU:CD1	2.29	0.62
1:C:54:ASN:ND2	1:C:56:ILE:H	1.99	0.60
1:D:117:ILE:O	2:D:1124:NPK:H34B	2.01	0.60
1:C:34:ILE:HD13	1:C:46:GLU:HG3	1.84	0.59
1:B:54:ASN:ND2	1:B:56:ILE:H	2.01	0.58
1:A:56:ILE:HD11	1:B:71:LYS:HE3	1.83	0.58
1:D:24:ASN:HD22	1:D:24:ASN:C	2.07	0.57
1:D:97:TRP:CZ2	1:D:116:GLY:HA3	2.40	0.57
1:A:88:ASN:HD21	1:A:90:LYS:HB2	1.70	0.56
1:B:117:ILE:O	2:B:1124:NPK:H34B	2.06	0.56
1:D:62:PRO:HD2	1:D:83:CYS:HB3	1.88	0.55
1:A:88:ASN:HD22	1:A:88:ASN:C	2.08	0.55
1:A:71:LYS:HE3	1:B:56:ILE:HD11	1.88	0.55
1:B:38:THR:OG1	1:B:40:THR:HG22	2.07	0.55
1:B:94:LYS:HD2	1:B:119:ILE:HD12	1.89	0.54
1:D:70:TRP:CZ2	2:D:1124:NPK:H8	2.42	0.54
1:B:17:ASN:CG	3:B:1125:NAG:C1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ARG:HA	4:D:1126:SO4:O2	2.09	0.53
1:A:69:ASN:HD21	1:B:54:ASN:HA	1.74	0.53
1:A:54:ASN:ND2	1:A:56:ILE:H	2.07	0.52
1:B:60:THR:HG23	4:B:1127:SO4:S	2.49	0.52
1:A:88:ASN:ND2	1:A:90:LYS:H	2.08	0.52
1:B:24:ASN:ND2	1:B:24:ASN:C	2.64	0.50
1:A:45:LYS:NZ	1:A:71:LYS:HB3	2.26	0.50
1:D:54:ASN:ND2	1:D:56:ILE:H	2.09	0.50
1:B:96:MET:HG2	1:B:117:ILE:HG22	1.94	0.49
1:C:54:ASN:HD21	1:C:56:ILE:HB	1.76	0.49
1:C:14:LEU:HD22	2:C:1124:NPK:C37	2.43	0.49
1:A:97:TRP:CZ2	1:A:116:GLY:HA3	2.49	0.48
1:C:19:THR:O	1:C:31:GLY:HA3	2.15	0.47
1:A:24:ASN:ND2	1:A:28:GLU:H	2.12	0.47
1:C:24:ASN:C	1:C:24:ASN:ND2	2.68	0.47
1:A:24:ASN:ND2	1:A:24:ASN:C	2.63	0.47
1:A:54:ASN:HD21	1:A:56:ILE:HB	1.80	0.47
1:D:83:CYS:HA	1:D:93:LEU:HD12	1.96	0.47
1:C:81:GLY:HA3	1:C:94:LYS:O	2.14	0.46
1:D:14:LEU:HD13	1:D:36:ALA:HB3	1.97	0.46
1:B:14:LEU:HG	1:B:14:LEU:O	2.16	0.46
1:A:117:ILE:HG12	1:D:117:ILE:HG21	1.98	0.46
1:C:97:TRP:CZ2	1:C:116:GLY:HA3	2.50	0.46
2:A:1124:NPK:H36	1:C:110:TRP:CB	2.46	0.45
1:B:86:ASP:OD2	1:B:86:ASP:C	2.55	0.45
1:A:88:ASN:C	1:A:88:ASN:ND2	2.70	0.44
1:D:93:LEU:HB2	1:D:120:PHE:HB2	1.98	0.44
1:A:71:LYS:HE3	1:A:71:LYS:HA	1.98	0.44
1:A:94:LYS:HD2	1:B:106:ILE:HD11	1.99	0.44
1:C:17:ASN:ND2	3:C:1125:NAG:N2	2.65	0.44
1:A:54:ASN:HA	1:B:69:ASN:HD21	1.82	0.44
1:C:24:ASN:ND2	1:C:28:GLU:H	2.15	0.44
1:C:54:ASN:HA	1:D:69:ASN:HD21	1.81	0.44
1:B:11:THR:HB	1:B:123:LEU:HG	1.98	0.44
1:C:88:ASN:ND2	1:C:90:LYS:H	2.17	0.43
2:A:1124:NPK:H36	1:C:110:TRP:HB3	2.00	0.43
1:B:14:LEU:HD21	1:B:37:VAL:HG22	2.00	0.43
1:C:56:ILE:HD13	1:C:56:ILE:N	2.33	0.43
1:C:14:LEU:HB2	2:C:1124:NPK:C38	2.49	0.42
2:A:1124:NPK:C36	1:C:110:TRP:HB3	2.49	0.42
1:C:40:THR:HG21	1:C:73:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TRP:CH2	2:A:1124:NPK:H8A	2.54	0.41
1:D:60:THR:N	4:D:1126:SO4:O2	2.49	0.41
1:A:14:LEU:HD22	2:A:1124:NPK:C37	2.51	0.41
1:A:40:THR:HG21	1:A:73:SER:HB2	2.01	0.41
1:B:105:ASP:CG	1:B:107:GLY:H	2.24	0.41
1:B:70:TRP:CH2	2:B:1124:NPK:H8A	2.56	0.41
1:A:14:LEU:HG	1:A:36:ALA:HB3	2.02	0.41
1:C:93:LEU:HB2	1:C:120:PHE:HB2	2.03	0.41
1:D:38:THR:OG1	1:D:40:THR:HB	2.21	0.41
1:D:17:ASN:ND2	3:D:1125:NAG:O5	2.45	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	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
1	B	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
1	C	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
1	D	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
All	All	480/492 (98%)	472 (98%)	8 (2%)	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	107/107 (100%)	99 (92%)	8 (8%)	13	9
1	B	106/107 (99%)	99 (93%)	7 (7%)	16	12
1	C	106/107 (99%)	94 (89%)	12 (11%)	6	3
1	D	106/107 (99%)	94 (89%)	12 (11%)	6	3
All	All	425/428 (99%)	386 (91%)	39 (9%)	9	5

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	24	ASN
1	A	54	ASN
1	A	71	LYS
1	A	88	ASN
1	A	94	LYS
1	A	111	LYS
1	A	123	LEU
1	B	24	ASN
1	B	26	ARG
1	B	40	THR
1	B	54	ASN
1	B	87	ARG
1	B	105	ASP
1	B	123	LEU
1	C	18	MET
1	C	24	ASN
1	C	26	ARG
1	C	34	ILE
1	C	45	LYS
1	C	54	ASN
1	C	56	ILE
1	C	58	LYS
1	C	88	ASN
1	C	93	LEU
1	C	117	ILE
1	C	122	ARG
1	D	3	LYS
1	D	14	LEU
1	D	24	ASN

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Mol	Chain	Res	Type
1	D	40	THR
1	D	54	ASN
1	D	71	LYS
1	D	87	ARG
1	D	93	LEU
1	D	94	LYS
1	D	105	ASP
1	D	122	ARG
1	D	123	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	54	ASN
1	A	69	ASN
1	A	88	ASN
1	B	17	ASN
1	B	24	ASN
1	B	54	ASN
1	B	69	ASN
1	C	17	ASN
1	C	24	ASN
1	C	54	ASN
1	C	69	ASN
1	C	88	ASN
1	D	17	ASN
1	D	24	ASN
1	D	54	ASN
1	D	69	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](#)

14 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
3	NAG	D	1125	1	14,14,15	1.37	2 (14%)	17,19,21	2.71	3 (17%)
4	SO4	A	1126	-	4,4,4	0.53	0	6,6,6	0.55	0
2	NPK	D	1124	-	32,36,36	3.09	10 (31%)	40,52,52	4.63	16 (40%)
2	NPK	A	1124	-	32,36,36	3.01	11 (34%)	40,52,52	4.90	17 (42%)
4	SO4	C	1127	-	4,4,4	0.14	0	6,6,6	0.72	0
2	NPK	C	1124	-	32,36,36	3.83	12 (37%)	40,52,52	4.66	14 (35%)
2	NPK	B	1124	-	32,36,36	3.19	9 (28%)	40,52,52	5.01	20 (50%)
4	SO4	D	1126	-	4,4,4	0.20	0	6,6,6	0.79	0
4	SO4	B	1126	-	4,4,4	0.54	0	6,6,6	1.10	0
4	SO4	B	1127	-	4,4,4	0.10	0	6,6,6	0.51	0
3	NAG	C	1125	1	14,14,15	1.20	1 (7%)	17,19,21	2.61	4 (23%)
4	SO4	A	1127	-	4,4,4	0.25	0	6,6,6	0.73	0
3	NAG	A	1125	1	14,14,15	1.82	4 (28%)	17,19,21	1.72	4 (23%)
3	NAG	B	1125	1	14,14,15	1.69	2 (14%)	17,19,21	2.72	8 (47%)

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	NAG	D	1125	1	-	2/6/23/26	0/1/1/1
2	NPK	D	1124	-	-	7/19/54/54	0/4/4/4
2	NPK	A	1124	-	-	9/19/54/54	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NPK	C	1124	-	-	9/19/54/54	0/4/4/4
2	NPK	B	1124	-	-	8/19/54/54	0/4/4/4
3	NAG	C	1125	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1125	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1125	1	-	2/6/23/26	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1124	NPK	C40-C35	13.28	1.57	1.39
2	D	1124	NPK	C40-C35	11.74	1.55	1.39
2	A	1124	NPK	C40-C35	10.17	1.53	1.39
2	C	1124	NPK	O44-C45	10.16	1.62	1.43
2	C	1124	NPK	O46-C45	10.02	1.62	1.43
2	C	1124	NPK	C40-C35	9.76	1.52	1.39
2	C	1124	NPK	C3-N2	-7.89	1.24	1.35
2	A	1124	NPK	C3-N2	-7.30	1.24	1.35
2	D	1124	NPK	C3-N2	-6.81	1.25	1.35
2	B	1124	NPK	C3-N2	-6.76	1.25	1.35
2	D	1124	NPK	O32-C30	5.71	1.45	1.34
2	B	1124	NPK	O32-C30	5.11	1.44	1.34
2	C	1124	NPK	O32-C30	4.97	1.44	1.34
3	B	1125	NAG	O5-C5	4.91	1.53	1.43
2	A	1124	NPK	C9-C10	-4.53	1.30	1.52
2	A	1124	NPK	O32-C30	4.26	1.42	1.34
2	A	1124	NPK	C3-N1	-4.16	1.33	1.40
3	A	1125	NAG	O5-C5	4.12	1.51	1.43
2	C	1124	NPK	C3-N1	-4.02	1.33	1.40
2	A	1124	NPK	O32-C33	-3.98	1.39	1.47
2	D	1124	NPK	C9-C10	-3.72	1.34	1.52
2	B	1124	NPK	C9-C10	-3.59	1.35	1.52
2	C	1124	NPK	C38-C37	3.50	1.48	1.39
2	C	1124	NPK	C9-C10	-3.49	1.35	1.52
3	A	1125	NAG	C4-C5	3.48	1.60	1.53
2	A	1124	NPK	C30-N1	-3.41	1.35	1.40
2	A	1124	NPK	C2-S1	-3.38	1.77	1.82
2	D	1124	NPK	C30-N1	-3.36	1.35	1.40
3	D	1125	NAG	O5-C5	3.32	1.50	1.43
2	D	1124	NPK	C38-C37	3.28	1.47	1.39
2	C	1124	NPK	C40-N40	-3.24	1.39	1.45
2	B	1124	NPK	C38-C37	3.19	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1124	NPK	C40-N40	-3.16	1.40	1.45
2	A	1124	NPK	C38-C37	3.11	1.47	1.39
2	C	1124	NPK	C2-S1	-3.07	1.77	1.82
2	B	1124	NPK	C30-N1	-2.98	1.35	1.40
2	D	1124	NPK	C3-N1	-2.83	1.35	1.40
2	D	1124	NPK	C34-C33	2.82	1.57	1.51
2	B	1124	NPK	C2-S1	-2.78	1.78	1.82
3	A	1125	NAG	C4-C3	2.73	1.59	1.52
3	D	1125	NAG	C8-C7	2.64	1.56	1.50
2	B	1124	NPK	C40-N40	-2.57	1.41	1.45
2	B	1124	NPK	C3-N1	-2.55	1.36	1.40
2	A	1124	NPK	O46-C45	2.47	1.47	1.43
3	B	1125	NAG	O4-C4	2.46	1.48	1.43
2	C	1124	NPK	C30-N1	-2.34	1.36	1.40
2	D	1124	NPK	O44-C45	2.30	1.47	1.43
3	A	1125	NAG	O4-C4	2.16	1.48	1.43
3	C	1125	NAG	C1-C2	-2.11	1.49	1.52
2	A	1124	NPK	C34-C33	2.10	1.55	1.51
2	C	1124	NPK	C34-C33	2.02	1.55	1.51

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1124	NPK	C2-C4-N2	-21.95	93.46	113.13
2	B	1124	NPK	C2-C4-N2	-20.51	94.75	113.13
2	D	1124	NPK	C2-C4-N2	-19.58	95.58	113.13
2	C	1124	NPK	C2-C4-N2	-18.57	96.49	113.13
2	C	1124	NPK	O32-C33-C35	15.03	130.89	107.65
2	B	1124	NPK	O32-C33-C35	14.97	130.79	107.65
2	A	1124	NPK	O32-C33-C35	13.27	128.16	107.65
2	D	1124	NPK	O32-C33-C35	12.56	127.06	107.65
2	B	1124	NPK	O32-C30-N1	9.48	121.90	110.81
2	C	1124	NPK	O32-C30-N1	8.57	120.83	110.81
2	D	1124	NPK	O32-C30-N1	7.45	119.52	110.81
3	D	1125	NAG	O5-C5-C6	7.42	118.83	107.20
2	B	1124	NPK	C8-C9-C10	7.38	142.47	113.76
2	D	1124	NPK	C33-O32-C30	7.08	123.91	115.31
3	B	1125	NAG	C1-O5-C5	-6.69	103.13	112.19
3	D	1125	NAG	C6-C5-C4	-6.64	97.45	113.00
2	D	1124	NPK	C8-C9-C10	6.29	138.22	113.76
3	C	1125	NAG	O5-C1-C2	-6.20	101.49	111.29
2	A	1124	NPK	O32-C30-N1	6.18	118.04	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1125	NAG	O5-C5-C6	5.89	116.44	107.20
2	B	1124	NPK	O32-C30-O31	-5.86	112.51	124.86
2	B	1124	NPK	C2-C4-C5	5.73	115.61	108.94
2	C	1124	NPK	C8-C9-C10	5.57	135.43	113.76
2	C	1124	NPK	O46-C45-O44	-5.54	99.22	108.08
2	A	1124	NPK	C33-O32-C30	5.49	121.98	115.31
2	D	1124	NPK	C8-C7-C2	-5.34	103.03	113.86
2	C	1124	NPK	O32-C30-O31	-5.32	113.65	124.86
2	A	1124	NPK	C8-C9-C10	5.08	133.55	113.76
3	C	1125	NAG	O5-C5-C6	-4.96	99.44	107.20
2	C	1124	NPK	C2-C4-C5	4.95	114.70	108.94
2	A	1124	NPK	O32-C30-O31	-4.91	114.50	124.86
2	C	1124	NPK	C33-O32-C30	4.84	121.19	115.31
2	A	1124	NPK	C9-C8-C7	-4.70	97.00	113.62
2	D	1124	NPK	C4-C2-S1	4.63	109.61	105.20
3	C	1125	NAG	C4-C3-C2	-4.51	104.41	111.02
2	D	1124	NPK	C4-C5-N1	-4.44	97.22	102.48
2	C	1124	NPK	C4-C5-N1	-4.26	97.43	102.48
3	C	1125	NAG	C6-C5-C4	-4.26	103.03	113.00
2	A	1124	NPK	C39-C40-C35	-4.23	120.03	123.13
2	D	1124	NPK	O32-C30-O31	-4.21	115.99	124.86
3	A	1125	NAG	O5-C1-C2	4.20	117.92	111.29
2	A	1124	NPK	C2-C4-C5	4.15	113.77	108.94
2	A	1124	NPK	C6-S1-C2	4.04	98.19	89.89
2	B	1124	NPK	C6-S1-C2	3.97	98.05	89.89
2	A	1124	NPK	C4-C5-N1	-3.96	97.79	102.48
2	B	1124	NPK	C33-O32-C30	3.85	119.98	115.31
2	B	1124	NPK	C45-O44-C37	3.83	110.31	105.34
2	A	1124	NPK	O46-C38-C37	-3.77	105.49	109.78
3	D	1125	NAG	C1-O5-C5	-3.76	107.10	112.19
2	A	1124	NPK	C45-O46-C38	3.71	110.17	105.34
2	A	1124	NPK	O54-N40-C40	3.69	125.34	119.03
2	C	1124	NPK	C5-N1-C30	3.64	129.70	120.62
2	D	1124	NPK	C7-C2-S1	3.49	122.29	112.64
3	B	1125	NAG	C2-N2-C7	-3.39	118.07	122.90
2	D	1124	NPK	C5-C6-S1	3.38	111.53	106.02
2	B	1124	NPK	C45-O46-C38	3.20	109.49	105.34
2	B	1124	NPK	O46-C38-C39	3.18	132.11	127.85
2	D	1124	NPK	C2-C4-C5	3.17	112.63	108.94
2	C	1124	NPK	C45-O46-C38	3.01	109.25	105.34
3	A	1125	NAG	C1-O5-C5	-2.97	108.17	112.19
2	B	1124	NPK	O46-C45-O44	-2.97	103.34	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1124	NPK	C6-C5-N1	-2.92	105.88	113.30
2	C	1124	NPK	C9-C8-C7	-2.90	103.37	113.62
3	A	1125	NAG	O3-C3-C2	-2.69	103.91	109.47
2	B	1124	NPK	C4-C5-N1	-2.57	99.44	102.48
2	A	1124	NPK	C4-C2-S1	2.55	107.64	105.20
3	B	1125	NAG	O6-C6-C5	-2.47	102.81	111.29
2	C	1124	NPK	C45-O44-C37	2.47	108.55	105.34
2	D	1124	NPK	C45-O44-C37	2.42	108.48	105.34
2	B	1124	NPK	O44-C37-C38	-2.39	107.06	109.78
2	B	1124	NPK	C5-N1-C30	2.37	126.55	120.62
3	B	1125	NAG	C8-C7-N2	2.31	120.01	116.10
2	B	1124	NPK	O54-N40-C40	-2.30	115.09	119.03
3	B	1125	NAG	C6-C5-C4	-2.26	107.72	113.00
2	A	1124	NPK	O31-C30-N1	2.24	127.17	123.01
2	D	1124	NPK	C5-N1-C30	2.24	126.20	120.62
2	B	1124	NPK	C39-C40-C35	-2.22	121.50	123.13
2	B	1124	NPK	O46-C38-C37	-2.21	107.27	109.78
2	D	1124	NPK	C6-S1-C2	2.19	94.39	89.89
2	A	1124	NPK	C36-C35-C40	2.17	119.53	116.55
2	B	1124	NPK	C5-C6-S1	2.14	109.52	106.02
2	D	1124	NPK	O44-C37-C38	-2.12	107.37	109.78
3	B	1125	NAG	O3-C3-C4	-2.10	105.48	110.35
3	A	1125	NAG	O3-C3-C4	2.09	115.18	110.35
2	C	1124	NPK	O54-N40-C40	2.04	122.53	119.03
3	B	1125	NAG	C3-C4-C5	-2.03	106.62	110.24

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1124	NPK	N1-C30-O32-C33
2	D	1124	NPK	O31-C30-O32-C33
2	D	1124	NPK	C35-C33-O32-C30
2	A	1124	NPK	S1-C2-C7-C8
2	A	1124	NPK	C4-C2-C7-C8
2	A	1124	NPK	N1-C30-O32-C33
2	A	1124	NPK	O31-C30-O32-C33
2	A	1124	NPK	C35-C33-O32-C30
2	A	1124	NPK	O32-C33-C35-C40
2	A	1124	NPK	C34-C33-C35-C40
2	C	1124	NPK	S1-C2-C7-C8
2	C	1124	NPK	C4-C2-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	1124	NPK	N1-C30-O32-C33
2	C	1124	NPK	O31-C30-O32-C33
2	C	1124	NPK	C35-C33-O32-C30
2	C	1124	NPK	O32-C33-C35-C40
2	C	1124	NPK	C34-C33-C35-C40
2	B	1124	NPK	S1-C2-C7-C8
2	B	1124	NPK	C4-C2-C7-C8
2	B	1124	NPK	N1-C30-O32-C33
2	B	1124	NPK	O31-C30-O32-C33
2	B	1124	NPK	C35-C33-O32-C30
2	B	1124	NPK	O32-C33-C35-C36
2	B	1124	NPK	O32-C33-C35-C40
3	B	1125	NAG	O5-C5-C6-O6
3	B	1125	NAG	C4-C5-C6-O6
3	D	1125	NAG	O5-C5-C6-O6
2	D	1124	NPK	C7-C8-C9-C10
3	C	1125	NAG	O5-C5-C6-O6
3	A	1125	NAG	O5-C5-C6-O6
3	A	1125	NAG	C4-C5-C6-O6
2	D	1124	NPK	O32-C33-C35-C36
2	A	1124	NPK	O32-C33-C35-C36
2	A	1124	NPK	C34-C33-C35-C36
2	C	1124	NPK	O32-C33-C35-C36
2	C	1124	NPK	C34-C33-C35-C36
2	D	1124	NPK	S1-C2-C7-C8
2	D	1124	NPK	O32-C33-C35-C40
3	D	1125	NAG	C4-C5-C6-O6
3	C	1125	NAG	C4-C5-C6-O6
2	B	1124	NPK	C7-C8-C9-C10

There are no ring outliers.

10 monomers are involved in 37 short contacts:

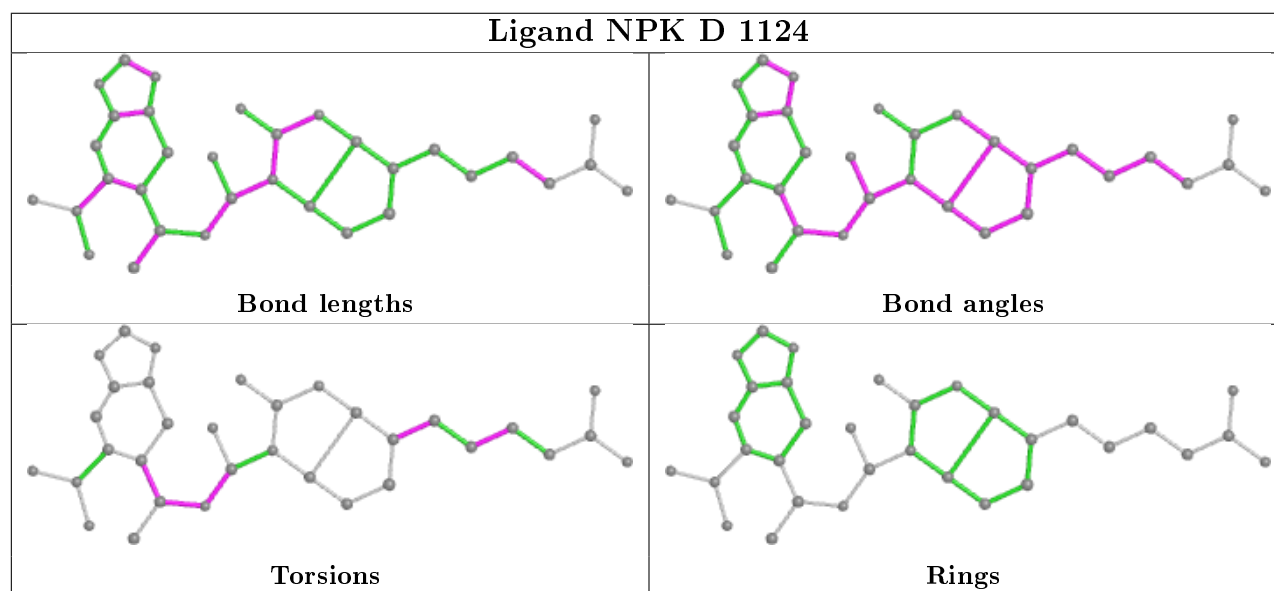
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1125	NAG	5	0
2	D	1124	NPK	3	0
2	A	1124	NPK	6	0
2	C	1124	NPK	4	0
2	B	1124	NPK	4	0
4	D	1126	SO4	3	0
4	B	1127	SO4	2	0
3	C	1125	NAG	6	0

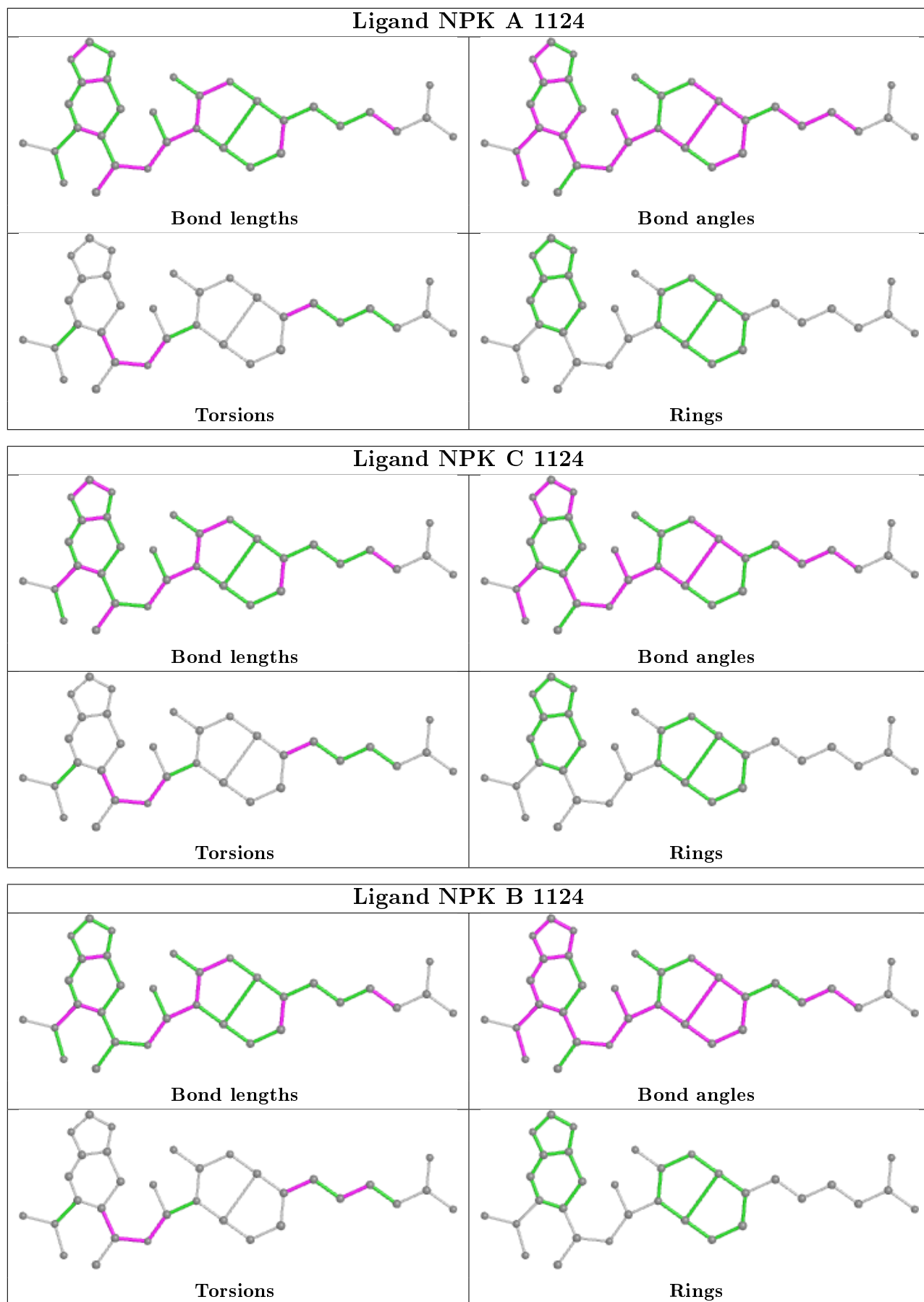
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1125	NAG	2	0
3	B	1125	NAG	2	0

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 [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	123/123 (100%)	-0.20	1 (0%) 86 85	14, 24, 42, 49	0
1	B	121/123 (98%)	-0.07	4 (3%) 46 45	12, 25, 46, 61	0
1	C	123/123 (100%)	-0.13	4 (3%) 46 45	14, 25, 44, 48	0
1	D	121/123 (98%)	-0.19	4 (3%) 46 45	12, 24, 46, 65	0
All	All	488/492 (99%)	-0.15	13 (2%) 54 53	12, 25, 45, 65	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	6.2
1	B	87	ARG	4.0
1	C	1	ALA	4.0
1	D	88	ASN	3.7
1	D	87	ARG	3.5
1	B	88	ASN	3.5
1	C	123	LEU	3.4
1	C	115	VAL	2.8
1	B	89	GLY	2.5
1	B	58	LYS	2.5
1	D	89	GLY	2.3
1	C	15	GLY	2.2
1	D	122	ARG	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](#)

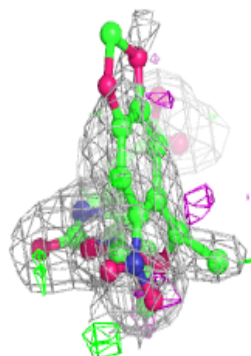
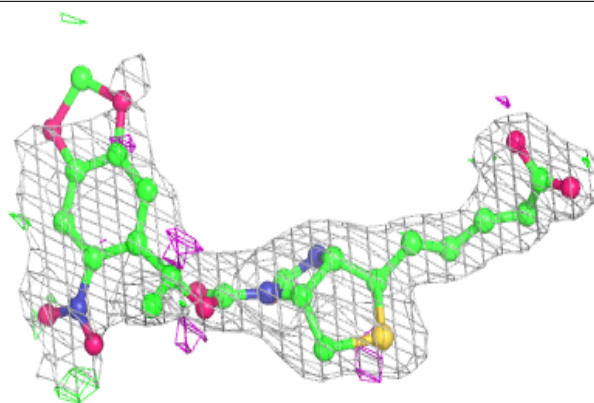
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	C	1125	14/15	0.81	0.23	47,61,67,67	0
2	NPK	C	1124	33/33	0.86	0.18	37,46,77,79	0
2	NPK	D	1124	33/33	0.89	0.15	27,44,70,73	0
2	NPK	A	1124	33/33	0.89	0.14	29,39,63,64	0
2	NPK	B	1124	33/33	0.90	0.14	25,40,67,69	0
3	NAG	A	1125	14/15	0.91	0.21	28,42,46,51	0
3	NAG	B	1125	14/15	0.91	0.14	36,44,45,47	0
3	NAG	D	1125	14/15	0.93	0.11	33,41,46,50	0
4	SO4	D	1126	5/5	0.94	0.11	62,64,65,65	0
4	SO4	B	1127	5/5	0.95	0.20	66,67,68,70	0
4	SO4	C	1127	5/5	0.97	0.20	55,57,58,59	0
4	SO4	A	1127	5/5	0.97	0.15	60,60,61,62	0
4	SO4	B	1126	5/5	0.99	0.09	40,40,43,47	0
4	SO4	A	1126	5/5	0.99	0.09	34,36,41,42	0

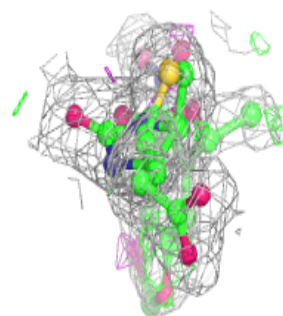
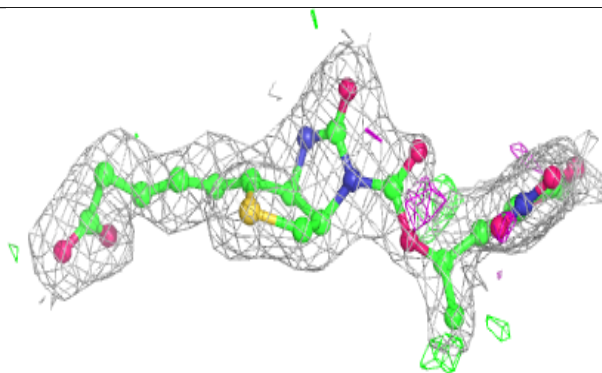
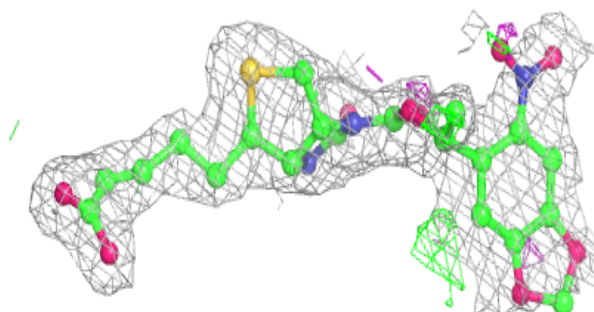
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NPK C 1124:

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

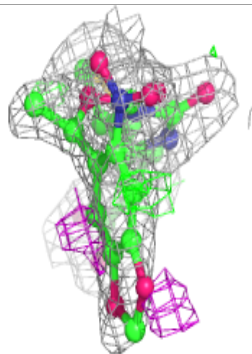
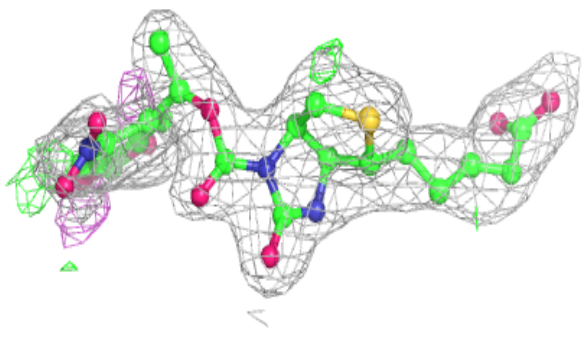
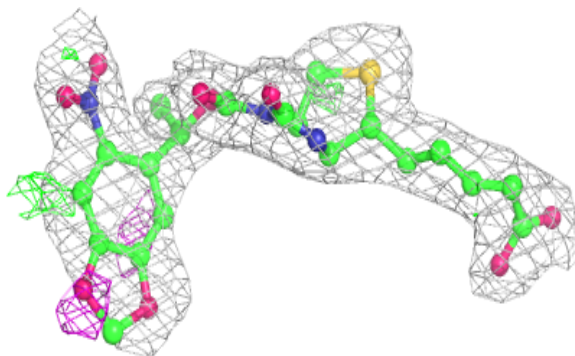
**Electron density around NPK D 1124:**

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

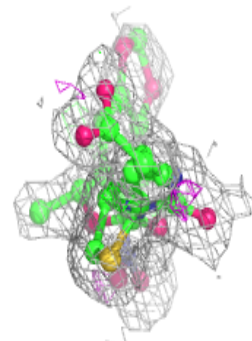
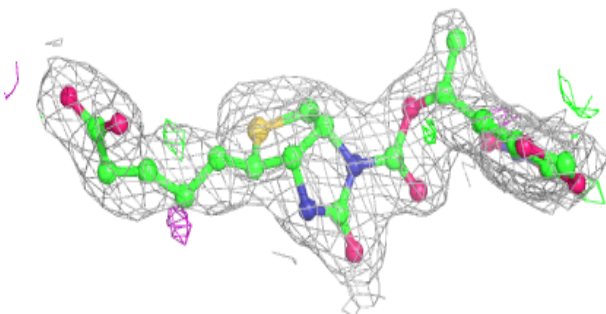
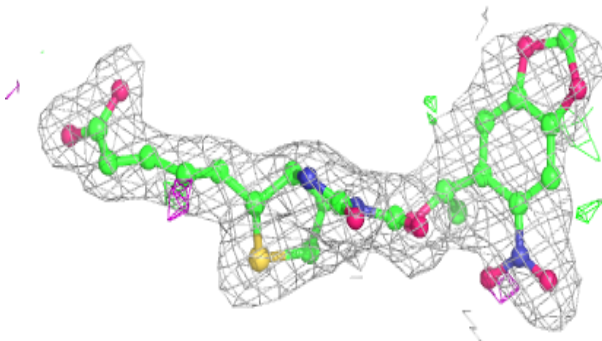


Electron density around NPK A 1124:

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

**Electron density around NPK B 1124:**

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



6.5 Other polymers

There are no such residues in this entry.