



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:32 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

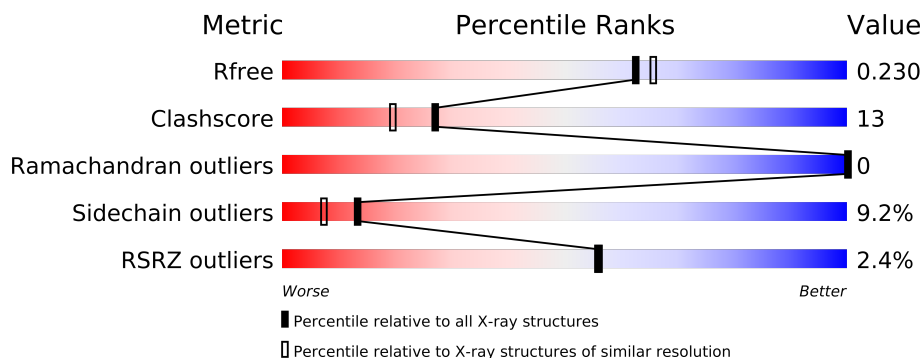
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	123	
1	B	123	
1	C	123	
1	D	123	

2 Entry composition i

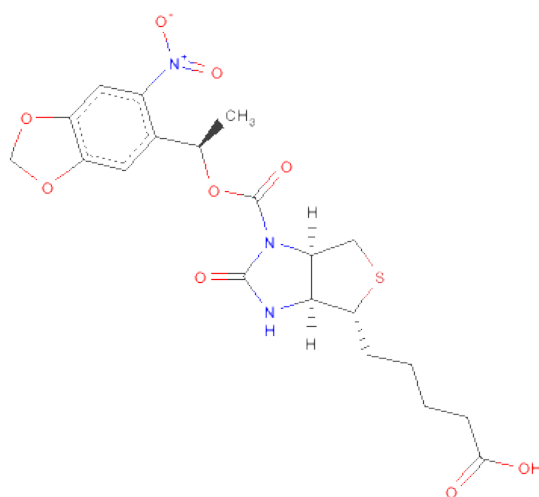
There are 5 unique types of molecules in this entry. The entry contains 4241 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	123	Total	C	N	O	S	0	0	0
			964	603	171	186	4			
1	B	121	Total	C	N	O	S	0	0	0
			948	594	166	184	4			
1	C	123	Total	C	N	O	S	0	0	0
			961	602	170	185	4			
1	D	121	Total	C	N	O	S	0	0	0
			948	594	166	184	4			

- 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).



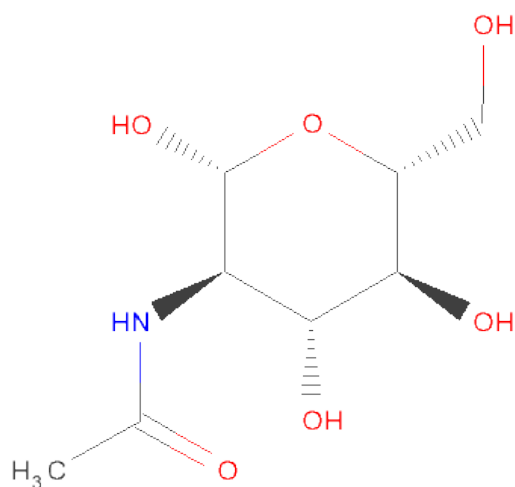
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	20	3	9	1		

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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



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

- Molecule 5 is water.

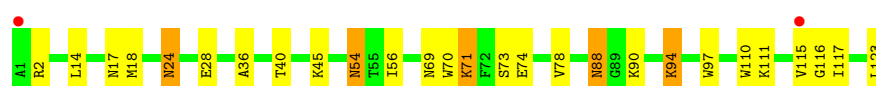
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	45	Total	O	0	0
			45	45		
5	C	57	Total	O	0	0
			57	57		
5	D	49	Total	O	0	0
			49	49		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

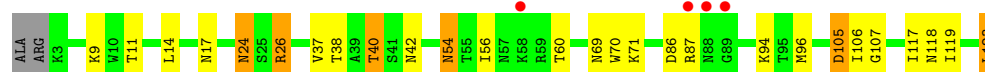
- Molecule 1: Avidin

Chain A: 



- Molecule 1: Avidin

Chain B: 



- Molecule 1: Avidin

Chain C: 



- Molecule 1: Avidin

Chain D: 



4 Data and refinement statistics

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)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.189 , 0.230 0.189 , 0.230	Depositor DCC
R_{free} test set	2228 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.2	EDS
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	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44247 reflections	Xtriage
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

Xtriage'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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (99) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:C	1:B:24:ASN:HD22	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:C	1:D:24:ASN:HD22	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:B:38:THR:OG1	1:B:40:THR:HG22	2.07	0.55
1:A:71:LYS:HE3	1:B:56:ILE:HD11	1.88	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
1:D:59:ARG:HA	4:D:1126:SO4:O2	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C	1:B:24:ASN:ND2	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:D:14:LEU:HD13	1:D:36:ALA:HB3	1.97	0.46
1:C:81:GLY:HA3	1:C:94:LYS:O	2.14	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:C:17:ASN:ND2	3:C:1125:NAG:N2	2.65	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:24:ASN:ND2	1:C:28:GLU:H	2.15	0.44
1:A:54:ASN:HA	1:B:69:ASN:HD21	1.82	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:C:56:ILE:HD13	1:C:56:ILE:N	2.33	0.43
1:B:14:LEU:HD21	1:B:37:VAL:HG22	2.00	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:38:THR:OG1	1:D:40:THR:HB	2.21	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:17:ASN:ND2	3:D:1125:NAG:O5	2.45	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	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 ⓘ

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%)	19	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	106/107 (99%)	99 (93%)	7 (7%)	24	16
1	C	106/107 (99%)	94 (89%)	12 (11%)	9	4
1	D	106/107 (99%)	94 (89%)	12 (11%)	9	4
All	All	425/428 (99%)	386 (91%)	39 (9%)	13	7

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
1	D	40	THR
1	D	54	ASN
1	D	71	LYS

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
2	NPK	A	1124	-	36,36,36	3.30	11 (30%)	52,52,52	3.92	23 (44%)
3	NAG	A	1125	1	12,14,15	1.84	5 (41%)	15,19,21	1.29	2 (13%)
4	SO4	A	1126	-	4,4,4	1.10	0	6,6,6	0.50	0
4	SO4	A	1127	-	4,4,4	0.20	0	6,6,6	0.76	0
2	NPK	B	1124	-	36,36,36	3.73	9 (25%)	52,52,52	4.11	24 (46%)
3	NAG	B	1125	1	12,14,15	1.67	2 (16%)	15,19,21	2.89	6 (40%)
4	SO4	B	1126	-	4,4,4	1.19	0	6,6,6	0.82	0
4	SO4	B	1127	-	4,4,4	0.34	0	6,6,6	0.68	0
2	NPK	C	1124	-	36,36,36	3.94	11 (30%)	52,52,52	3.64	20 (38%)
3	NAG	C	1125	1	12,14,15	1.25	1 (8%)	15,19,21	2.41	3 (20%)
4	SO4	C	1127	-	4,4,4	0.35	0	6,6,6	0.85	0
2	NPK	D	1124	-	36,36,36	3.51	10 (27%)	52,52,52	3.84	23 (44%)
3	NAG	D	1125	1	12,14,15	1.27	2 (16%)	15,19,21	3.50	3 (20%)
4	SO4	D	1126	-	4,4,4	0.41	0	6,6,6	0.90	0

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	NPK	A	1124	-	-	0/23/54/54	0/0/4/4
3	NAG	A	1125	1	-	0/6/23/26	0/1/1/1
4	SO4	A	1126	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1127	-	-	0/0/0/0	0/0/0/0
2	NPK	B	1124	-	-	1/23/54/54	0/0/4/4
3	NAG	B	1125	1	-	0/6/23/26	0/1/1/1
4	SO4	B	1126	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1127	-	-	0/0/0/0	0/0/0/0
2	NPK	C	1124	-	-	0/23/54/54	0/0/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1125	1	-	0/6/23/26	0/1/1/1
4	SO4	C	1127	-	-	0/0/0/0	0/0/0/0
2	NPK	D	1124	-	-	0/23/54/54	0/0/4/4
3	NAG	D	1125	1	-	0/6/23/26	0/1/1/1
4	SO4	D	1126	-	-	0/0/0/0	0/0/0/0

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1124	NPK	C40-C35	18.33	1.57	1.40
2	D	1124	NPK	C40-C35	16.17	1.55	1.40
2	A	1124	NPK	C40-C35	13.96	1.53	1.40
2	C	1124	NPK	C40-C35	13.39	1.52	1.40
2	C	1124	NPK	O44-C45	9.78	1.62	1.43
2	C	1124	NPK	O46-C45	9.65	1.62	1.43
2	C	1124	NPK	C3-N2	-8.47	1.24	1.35
2	A	1124	NPK	C3-N2	-7.83	1.24	1.35
2	D	1124	NPK	C3-N2	-7.30	1.25	1.35
2	B	1124	NPK	C3-N2	-7.25	1.25	1.35
2	D	1124	NPK	O32-C30	5.59	1.45	1.34
2	A	1124	NPK	C9-C10	-5.57	1.30	1.52
2	B	1124	NPK	O32-C30	5.00	1.44	1.34
2	C	1124	NPK	O32-C30	4.85	1.44	1.34
2	D	1124	NPK	C9-C10	-4.59	1.34	1.52
2	B	1124	NPK	C9-C10	-4.42	1.35	1.52
2	C	1124	NPK	C40-N40	-4.30	1.39	1.46
2	C	1124	NPK	C9-C10	-4.30	1.35	1.52
3	B	1125	NAG	O5-C5	4.30	1.53	1.45
2	D	1124	NPK	C40-N40	-4.21	1.40	1.46
2	A	1124	NPK	O32-C30	4.16	1.42	1.34
2	A	1124	NPK	C3-N1	-3.88	1.33	1.40
2	A	1124	NPK	O32-C33	-3.80	1.39	1.46
2	C	1124	NPK	C3-N1	-3.75	1.33	1.40
2	B	1124	NPK	C40-N40	-3.50	1.41	1.46
3	A	1125	NAG	O5-C5	3.44	1.51	1.45
3	A	1125	NAG	C4-C5	3.34	1.60	1.53
2	A	1124	NPK	C30-N1	-3.26	1.35	1.40
2	C	1124	NPK	C38-C37	3.24	1.48	1.39
2	D	1124	NPK	C30-N1	-3.20	1.35	1.40
3	C	1125	NAG	O5-C5	-3.15	1.39	1.45
2	D	1124	NPK	C38-C37	3.03	1.47	1.39
2	B	1124	NPK	C38-C37	2.95	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1124	NPK	C2-S1	-2.95	1.77	1.82
2	A	1124	NPK	C38-C37	2.87	1.47	1.39
2	B	1124	NPK	C30-N1	-2.84	1.35	1.40
2	C	1124	NPK	C2-S1	-2.67	1.77	1.82
2	D	1124	NPK	C3-N1	-2.65	1.35	1.40
3	A	1125	NAG	C4-C3	2.59	1.59	1.52
3	D	1125	NAG	C8-C7	2.58	1.56	1.50
3	D	1125	NAG	O5-C5	2.57	1.50	1.45
2	D	1124	NPK	C34-C33	2.43	1.57	1.51
2	B	1124	NPK	C2-S1	-2.41	1.78	1.82
3	B	1125	NAG	O4-C4	2.41	1.48	1.43
2	B	1124	NPK	C3-N1	-2.39	1.36	1.40
2	A	1124	NPK	O46-C45	2.38	1.47	1.43
2	A	1124	NPK	C40-N40	-2.38	1.42	1.46
2	C	1124	NPK	C30-N1	-2.24	1.36	1.40
2	D	1124	NPK	O44-C45	2.22	1.47	1.43
3	A	1125	NAG	O4-C4	2.11	1.48	1.43
3	A	1125	NAG	C2-N2	2.03	1.48	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1124	NPK	O32-C33-C35	14.82	130.89	107.89
2	B	1124	NPK	O32-C33-C35	14.75	130.79	107.89
2	A	1124	NPK	C2-C4-N2	-13.93	93.46	113.27
2	A	1124	NPK	O32-C33-C35	13.06	128.16	107.89
2	B	1124	NPK	C2-C4-N2	-13.02	94.75	113.27
2	D	1124	NPK	C2-C4-N2	-12.44	95.58	113.27
2	D	1124	NPK	O32-C33-C35	12.35	127.06	107.89
2	C	1124	NPK	C2-C4-N2	-11.80	96.49	113.27
3	D	1125	NAG	O5-C5-C6	11.29	118.83	106.98
3	B	1125	NAG	O5-C5-C6	9.02	116.44	106.98
2	B	1124	NPK	O32-C30-N1	8.55	121.90	110.87
2	A	1124	NPK	C36-C35-C33	-8.03	106.95	120.82
2	B	1124	NPK	C40-C35-C33	8.01	133.91	124.69
2	B	1124	NPK	C8-C9-C10	7.75	142.47	113.28
2	C	1124	NPK	O32-C30-N1	7.73	120.83	110.87
3	C	1125	NAG	O5-C5-C6	-7.19	99.44	106.98
2	D	1124	NPK	C9-C10-C11	-7.13	95.09	114.51
2	D	1124	NPK	C40-C35-C33	7.11	132.88	124.69
2	B	1124	NPK	C36-C35-C33	-6.99	108.75	120.82
2	A	1124	NPK	C40-C35-C33	6.91	132.64	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1124	NPK	O32-C30-N1	6.71	119.52	110.87
2	D	1124	NPK	C36-C35-C33	-6.65	109.34	120.82
2	D	1124	NPK	C8-C9-C10	6.62	138.22	113.28
3	D	1125	NAG	C6-C5-C4	-6.43	97.45	113.00
2	D	1124	NPK	C33-O32-C30	6.26	123.91	115.69
2	B	1124	NPK	O32-C30-O31	-5.92	112.51	124.67
2	C	1124	NPK	C8-C9-C10	5.88	135.43	113.28
2	B	1124	NPK	C9-C10-C11	-5.62	99.20	114.51
2	A	1124	NPK	O32-C30-N1	5.56	118.04	110.87
2	A	1124	NPK	C8-C9-C10	5.38	133.55	113.28
2	C	1124	NPK	O32-C30-O31	-5.37	113.65	124.67
2	C	1124	NPK	O46-C45-O44	-5.11	99.22	108.09
2	A	1124	NPK	C9-C10-C11	-5.02	100.84	114.51
2	A	1124	NPK	O32-C30-O31	-4.95	114.50	124.67
2	A	1124	NPK	C39-C40-C35	-4.80	120.03	123.08
2	A	1124	NPK	C33-O32-C30	4.79	121.98	115.69
2	A	1124	NPK	C9-C8-C7	-4.57	97.00	113.64
2	D	1124	NPK	C8-C7-C2	-4.33	103.03	113.40
2	D	1124	NPK	O32-C30-O31	-4.23	115.99	124.67
2	C	1124	NPK	C33-O32-C30	4.19	121.19	115.69
3	C	1125	NAG	C6-C5-C4	-4.13	103.03	113.00
2	C	1124	NPK	C5-N1-C30	4.07	129.70	120.13
2	D	1124	NPK	C39-C40-N40	-4.05	111.76	115.82
2	B	1124	NPK	C2-C4-C5	4.00	115.61	108.55
2	C	1124	NPK	C36-C35-C33	-3.95	114.00	120.82
2	D	1124	NPK	C7-C2-S1	3.93	122.29	112.72
2	C	1124	NPK	C35-C40-N40	3.77	125.38	119.62
2	C	1124	NPK	C9-C10-C11	-3.76	104.26	114.51
2	C	1124	NPK	C40-C35-C33	3.76	129.02	124.69
2	C	1124	NPK	C39-C40-N40	-3.69	112.12	115.82
2	A	1124	NPK	C35-C40-N40	3.67	125.22	119.62
2	D	1124	NPK	C35-C40-N40	3.65	125.20	119.62
2	B	1124	NPK	C6-C5-N1	-3.57	105.88	113.54
2	C	1124	NPK	C2-C4-C5	3.49	114.70	108.55
2	D	1124	NPK	C4-C2-S1	3.46	109.61	105.29
2	B	1124	NPK	C45-O44-C37	3.44	110.31	105.36
2	A	1124	NPK	O46-C38-C37	-3.36	105.49	109.78
2	A	1124	NPK	C45-O46-C38	3.34	110.17	105.36
2	B	1124	NPK	C33-O32-C30	3.27	119.98	115.69
2	A	1124	NPK	C6-S1-C2	3.26	98.19	90.94
2	B	1124	NPK	C6-S1-C2	3.20	98.05	90.94
2	A	1124	NPK	C40-C39-C38	-3.12	116.53	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1124	NPK	C4-N2-C3	3.10	116.96	113.01
2	D	1124	NPK	C40-C39-C38	-3.03	116.62	119.98
3	B	1125	NAG	C2-N2-C7	-2.99	118.07	123.09
2	A	1124	NPK	N2-C3-N1	-2.97	105.94	107.41
2	A	1124	NPK	C2-C4-C5	2.96	113.77	108.55
2	C	1124	NPK	C3-N1-C30	-2.94	120.30	126.71
2	B	1124	NPK	O46-C38-C39	2.94	132.11	127.85
2	B	1124	NPK	O55-N40-C40	2.90	126.19	117.25
2	B	1124	NPK	C45-O46-C38	2.87	109.49	105.36
3	C	1125	NAG	C4-C3-C2	-2.82	104.41	111.32
2	C	1124	NPK	C9-C8-C7	-2.82	103.37	113.64
2	D	1124	NPK	C5-C6-S1	2.81	111.53	105.95
2	B	1124	NPK	O46-C45-O44	-2.74	103.34	108.09
2	B	1124	NPK	C5-N1-C30	2.73	126.55	120.13
2	C	1124	NPK	C45-O46-C38	2.70	109.25	105.36
2	B	1124	NPK	C35-C40-N40	2.64	123.65	119.62
2	A	1124	NPK	C3-N1-C30	-2.62	120.99	126.71
2	D	1124	NPK	C5-N1-C30	2.58	126.20	120.13
2	D	1124	NPK	C3-N1-C30	-2.49	121.28	126.71
3	B	1125	NAG	O6-C6-C5	-2.49	102.81	111.36
2	B	1124	NPK	C39-C40-C35	-2.48	121.50	123.08
3	A	1125	NAG	O3-C3-C2	-2.47	103.91	109.09
2	B	1124	NPK	C3-N1-C30	-2.45	121.37	126.71
2	D	1124	NPK	C6-C5-N1	-2.37	108.45	113.54
2	D	1124	NPK	C2-C4-C5	2.31	112.63	108.55
2	A	1124	NPK	C5-N1-C30	2.30	125.52	120.13
2	B	1124	NPK	O12-C11-O11	-2.27	117.53	123.30
2	D	1124	NPK	N2-C3-N1	-2.25	106.30	107.41
2	A	1124	NPK	O54-N40-C40	2.22	125.34	119.33
2	C	1124	NPK	C45-O44-C37	2.22	108.55	105.36
2	A	1124	NPK	O31-C30-N1	2.19	127.17	122.94
2	D	1124	NPK	O12-C11-O11	-2.19	117.74	123.30
3	B	1125	NAG	C6-C5-C4	-2.19	107.72	113.00
3	B	1125	NAG	O3-C3-C4	-2.17	105.48	110.35
2	D	1124	NPK	C45-O44-C37	2.17	108.48	105.36
3	A	1125	NAG	O3-C3-C4	2.15	115.18	110.35
2	B	1124	NPK	O44-C37-C38	-2.13	107.06	109.78
2	B	1124	NPK	N2-C3-N1	2.10	108.45	107.41
2	C	1124	NPK	C7-C2-C4	-2.08	109.19	115.18
2	C	1124	NPK	O12-C11-O11	-2.07	118.04	123.30
3	D	1125	NAG	O5-C5-C4	2.04	113.24	110.65
3	B	1125	NAG	C3-C4-C5	-2.01	106.62	110.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1124	NPK	C35-C40-N40-O55

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	123/123 (100%)	-0.17	2 (1%) 68 69	14, 24, 42, 49	0
1	B	121/123 (98%)	-0.09	4 (3%) 44 44	12, 25, 46, 61	0
1	C	123/123 (100%)	-0.02	4 (3%) 44 44	14, 25, 44, 48	0
1	D	121/123 (98%)	-0.11	2 (1%) 67 67	12, 24, 46, 65	0
All	All	488/492 (99%)	-0.10	12 (2%) 56 54	12, 25, 45, 65	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	5.5
1	C	1	ALA	4.1
1	B	87	ARG	3.9
1	C	123	LEU	3.5
1	B	88	ASN	3.1
1	D	87	ARG	3.1
1	C	15	GLY	2.9
1	D	88	ASN	2.7
1	C	115	VAL	2.7
1	B	58	LYS	2.5
1	A	115	VAL	2.2
1	B	89	GLY	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	1125	14/15	0.21	1.60	28,42,46,51	0
2	NPK	D	1124	33/33	0.15	1.45	27,44,70,73	0
2	NPK	B	1124	33/33	0.15	1.34	25,40,67,69	0
2	NPK	C	1124	33/33	0.18	1.32	37,46,77,79	0
2	NPK	A	1124	33/33	0.14	1.12	29,39,63,64	0
3	NAG	B	1125	14/15	0.14	1.05	36,44,45,47	0
3	NAG	C	1125	14/15	0.25	0.81	47,61,67,67	0
3	NAG	D	1125	14/15	0.13	0.49	33,41,46,50	0
4	SO4	B	1126	5/5	0.09	-0.27	40,40,43,47	0
4	SO4	C	1127	5/5	0.13	-0.31	55,57,58,59	0
4	SO4	B	1127	5/5	0.16	-0.60	66,67,68,70	0
4	SO4	A	1127	5/5	0.10	-0.63	60,60,61,62	0
4	SO4	A	1126	5/5	0.08	-0.90	34,36,41,42	0
4	SO4	D	1126	5/5	0.07	-1.73	62,64,65,65	0

6.5 Other polymers

There are no such residues in this entry.