



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:25 PM BST

PDB ID : 2WNL
Title : CRYSTAL STRUCTURE OF APLYSIA ACHBP IN COMPLEX WITH AN-
ABASEINE
Authors : Sulzenbacher, G.; Hibbs, R.; Shi, J.; Talley, T.; Conrod, S.; Kem, W.; Taylor,
P.; Marchot, P.; Bourne, Y.
Deposited on : 2009-07-09
Resolution : 2.70 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
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

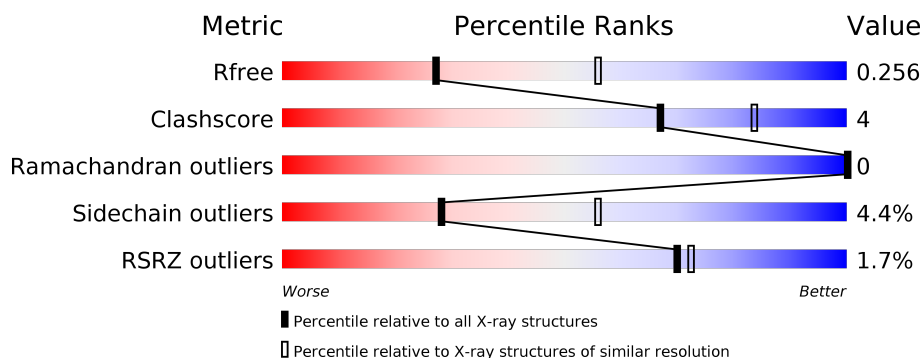
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	227	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>
1	B	227	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>7%</div> </div> </div>
1	C	227	<div> <div>0%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>
1	D	227	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>
1	E	227	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
1	F	227	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	227	<div><div><div>%</div><div><div></div><div>80%</div><div>11%</div><div>7%</div></div></div></div>
1	H	227	<div><div><div>2%</div><div><div></div><div>82%</div><div>11%</div><div>7%</div></div></div></div>
1	I	227	<div><div><div>2%</div><div><div></div><div>79%</div><div>13%</div><div>7%</div></div></div></div>
1	J	227	<div><div><div></div><div><div></div><div>79%</div><div>13%</div><div>7%</div></div></div></div>

2 Entry composition

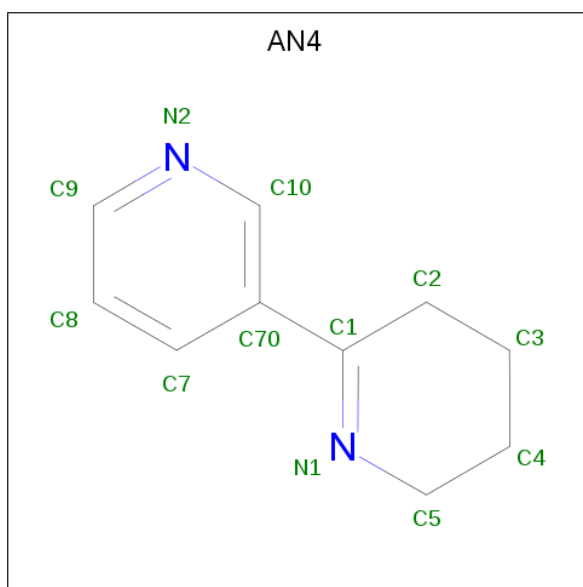
There are 7 unique types of molecules in this entry. The entry contains 17412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SOLUBLE ACETYLCHOLINE RECEPTOR.

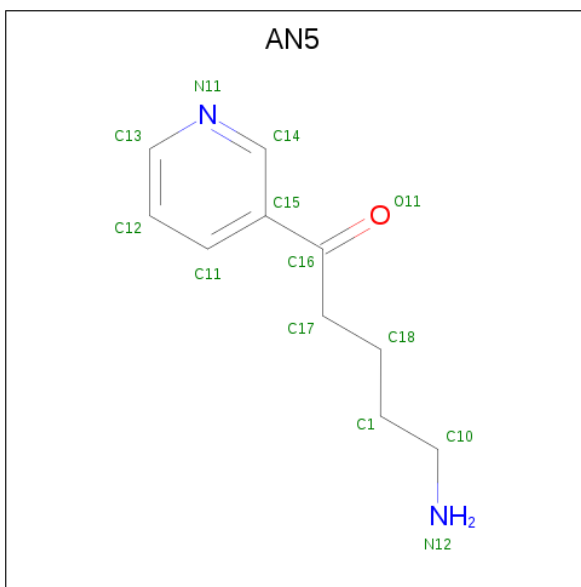
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	2	0
			1713	1079	283	342	9			
1	B	211	Total	C	N	O	S	0	1	0
			1690	1065	281	336	8			
1	C	209	Total	C	N	O	S	0	1	0
			1677	1058	279	332	8			
1	D	212	Total	C	N	O	S	0	1	0
			1697	1071	282	335	9			
1	E	214	Total	C	N	O	S	0	0	0
			1708	1075	281	343	9			
1	F	211	Total	C	N	O	S	0	1	0
			1692	1068	281	334	9			
1	G	210	Total	C	N	O	S	0	0	0
			1677	1057	277	335	8			
1	H	212	Total	C	N	O	S	0	0	0
			1692	1067	279	337	9			
1	I	211	Total	C	N	O	S	0	1	0
			1692	1068	281	334	9			
1	J	212	Total	C	N	O	S	0	1	0
			1697	1071	282	335	9			

- Molecule 2 is 3,4,5,6-tetrahydro-2,3'-bipyridine (three-letter code: AN4) (formula: C₁₀H₁₂N₂).



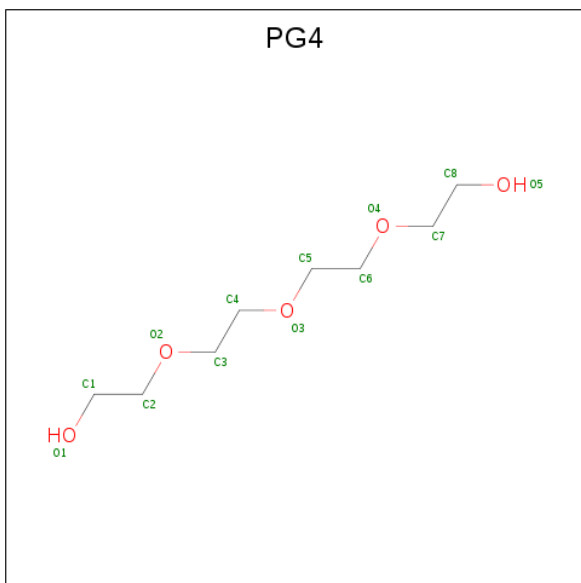
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	1
			12	10	2		
2	B	1	Total	C	N	0	0
			12	10	2		
2	E	1	Total	C	N	0	0
			12	10	2		
2	G	1	Total	C	N	0	0
			12	10	2		
2	J	1	Total	C	N	0	0
			12	10	2		

- Molecule 3 is 5-amino-1-pyridin-3-ylpentan-1-one (three-letter code: AN5) (formula: $C_{10}H_{14}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			13	10	2	1		
3	D	1	Total	C	N	O	0	0
			13	10	2	1		
3	F	1	Total	C	N	O	0	0
			13	10	2	1		
3	I	1	Total	C	N	O	0	0
			13	10	2	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).

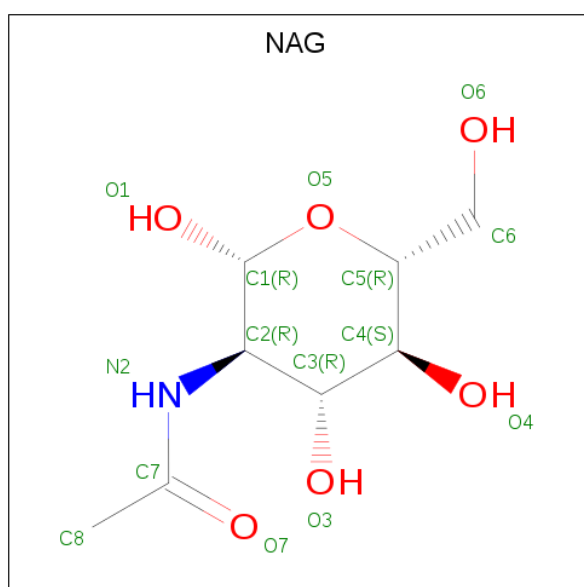


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	8	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

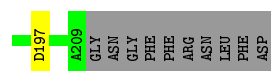
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



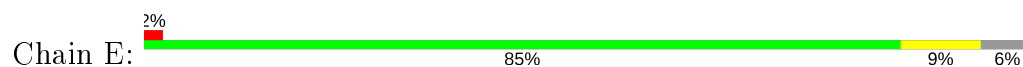
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

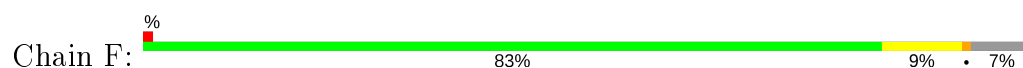
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	47	Total 47	O 47	0	0
7	B	42	Total 42	O 42	0	0
7	C	32	Total 32	O 32	0	0
7	D	23	Total 23	O 23	0	0
7	E	23	Total 23	O 23	0	0
7	F	26	Total 26	O 26	0	0
7	G	27	Total 27	O 27	0	0
7	H	27	Total 27	O 27	0	0
7	I	29	Total 29	O 29	0	0
7	J	31	Total 31	O 31	0	0



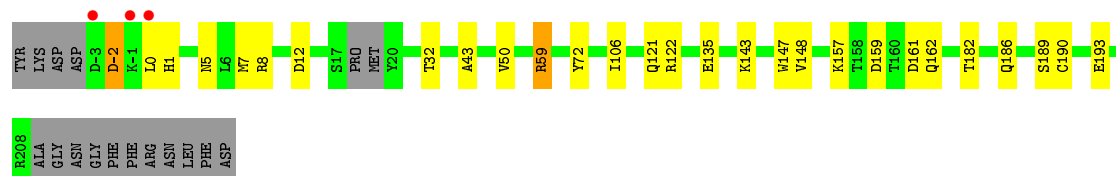
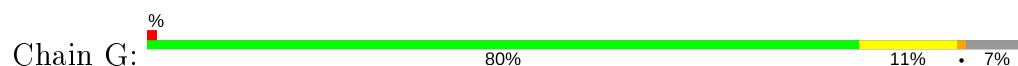
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



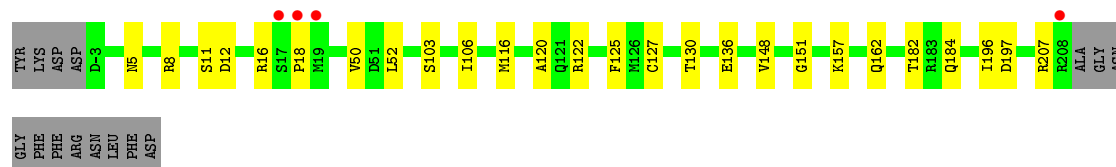
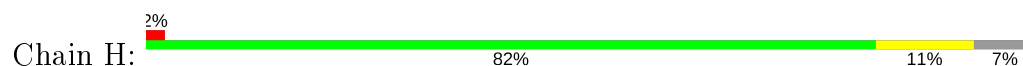
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



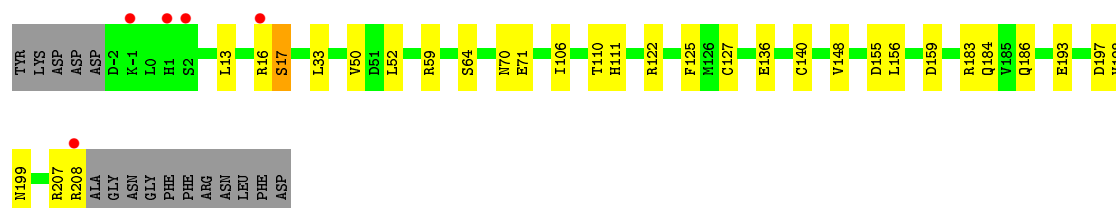
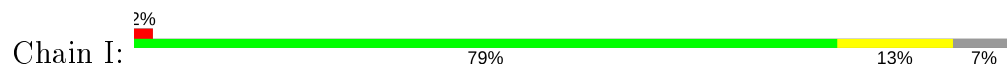
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



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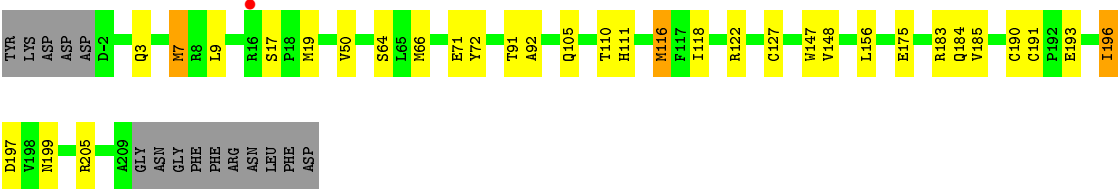
● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain J:

79%

13%

7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.25Å 125.77Å 257.00Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	258.20 – 2.70 69.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (258.20-2.70) 99.5 (69.78-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.202 , 0.251 0.212 , 0.256	Depositor DCC
R_{free} test set	2199 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17412	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: AN4, AN5, MG, NAG, PG4

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	0.40	0/1760	0.61	1/2399 (0.0%)
1	B	0.40	0/1732	0.60	0/2359
1	C	0.38	0/1719	0.60	0/2341
1	D	0.38	0/1741	0.60	0/2373
1	E	0.37	0/1749	0.60	1/2384 (0.0%)
1	F	0.41	0/1736	0.62	1/2365 (0.0%)
1	G	0.38	0/1716	0.59	0/2337
1	H	0.40	0/1733	0.60	0/2362
1	I	0.40	0/1736	0.60	1/2366 (0.0%)
1	J	0.37	0/1741	0.59	0/2373
All	All	0.39	0/17363	0.60	4/23659 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	140	CYS	CA-CB-SG	-6.83	101.71	114.00
1	I	140	CYS	CA-CB-SG	-5.33	104.41	114.00
1	A	140	CYS	CA-CB-SG	-5.33	104.41	114.00
1	E	122	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	190	CYS	Peptide
1	D	190	CYS	Peptide

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	1713	0	1642	19	0
1	B	1690	0	1622	21	0
1	C	1677	0	1613	12	0
1	D	1697	0	1635	14	0
1	E	1708	0	1628	8	0
1	F	1692	0	1629	18	0
1	G	1677	0	1604	13	0
1	H	1692	0	1620	10	0
1	I	1692	0	1630	14	0
1	J	1697	0	1635	20	0
2	A	12	0	12	2	0
2	B	12	0	12	2	0
2	E	12	0	12	0	0
2	G	12	0	12	2	0
2	J	12	0	12	4	0
3	A	13	0	14	1	0
3	D	13	0	14	0	0
3	F	13	0	14	3	0
3	I	13	0	14	0	0
4	C	13	0	18	1	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
6	E	14	0	13	1	0
6	F	14	0	13	0	0
6	H	14	0	13	0	0
7	A	47	0	0	0	0
7	B	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	32	0	0	0	0
7	D	23	0	0	0	0
7	E	23	0	0	0	0
7	F	26	0	0	0	0
7	G	27	0	0	0	0
7	H	27	0	0	0	0
7	I	29	0	0	0	0
7	J	31	0	0	0	0
All	All	17412	0	16431	131	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 4.

All (131) 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:F:93:TYR:HB3	3:F:300:AN5:H14	1.45	0.97
1:A:93:TYR:HB3	3:A:301[A]:AN5:H14	1.54	0.88
1:J:185:VAL:HG22	1:J:196:ILE:HD13	1.58	0.86
1:F:18:PRO:HG2	1:J:7:MET:SD	2.18	0.84
1:C:12:ASP:OD2	1:C:72:TYR:OH	1.96	0.81
1:A:93:TYR:HB3	2:A:300[B]:AN4:H10	1.65	0.78
1:I:184:GLN:NE2	1:I:197:ASP:OD2	2.17	0.77
1:A:18:PRO:HG2	1:E:7:MET:SD	2.25	0.76
1:B:59:ARG:NH2	1:B:159:ASP:OD2	2.19	0.76
1:J:190:CYS:SG	2:J:300:AN4:H22C	2.30	0.71
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.31	0.70
1:E:29:LEU:HD21	1:E:60:TRP:HB2	1.72	0.69
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.32	0.69
1:F:59:ARG:NH1	1:F:159:ASP:OD1	2.31	0.64
1:D:5:ASN:O	1:D:8:ARG:HB2	1.99	0.63
1:J:184:GLN:NE2	1:J:199:ASN:HB2	2.13	0.63
1:D:59:ARG:NH1	1:D:159:ASP:OD2	2.28	0.61
1:B:186:GLN:HG3	1:F:185:VAL:HB	1.81	0.61
1:H:12:ASP:O	1:H:16:ARG:HB2	2.01	0.61
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.41	0.61
1:J:184:GLN:NE2	1:J:197:ASP:OD1	2.33	0.61
1:G:59:ARG:NH2	1:G:159:ASP:OD2	2.34	0.61
1:C:191:CYS:HB3	1:C:193:GLU:OE2	2.01	0.60
1:J:190:CYS:SG	1:J:191:CYS:N	2.75	0.60
1:D:29:LEU:HD11	1:D:62:LEU:CD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:LEU:HD21	1:D:67:TRP:CE2	2.37	0.59
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.42	0.59
1:A:93:TYR:CD2	2:A:300[B]:AN4:H21C	2.37	0.59
1:J:190:CYS:SG	2:J:300:AN4:C2	2.91	0.59
1:H:50:VAL:HG21	1:H:127:CYS:SG	2.43	0.59
1:F:106:ILE:HB	1:G:148:VAL:HG11	1.84	0.58
1:B:105:GLN:HE21	1:B:105:GLN:HA	1.67	0.58
1:A:190:CYS:SG	1:A:191:CYS:N	2.78	0.57
1:D:8:ARG:HG3	1:D:8:ARG:HH11	1.70	0.57
1:J:175:GLU:OE2	1:J:205:ARG:NH1	2.38	0.56
1:G:5:ASN:OD1	1:G:8:ARG:NH2	2.38	0.56
1:G:43:ALA:HA	1:G:50:VAL:HG22	1.86	0.56
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.46	0.56
1:B:190:CYS:SG	1:B:191:CYS:N	2.80	0.55
1:H:5:ASN:OD1	1:H:8:ARG:NH2	2.40	0.55
1:C:50:VAL:CG2	1:C:127:CYS:SG	2.94	0.55
1:H:106:ILE:HG21	1:I:148:VAL:HG21	1.89	0.54
1:F:93:TYR:CB	3:F:300:AN5:H14	2.30	0.54
1:A:106:ILE:HB	1:B:148:VAL:HG11	1.89	0.54
1:B:5:ASN:OD1	1:B:8:ARG:NH2	2.40	0.53
1:J:147:TRP:O	2:J:300:AN4:N1	2.42	0.53
1:E:50:VAL:CG2	1:E:127:CYS:SG	2.95	0.53
1:H:184:GLN:NE2	1:H:197:ASP:OD2	2.36	0.53
1:D:9:LEU:HD11	1:D:67:TRP:CG	2.44	0.52
1:D:0:LEU:O	1:D:4:ALA:HB2	2.08	0.52
1:I:59:ARG:NH2	1:I:159:ASP:OD2	2.42	0.52
1:J:50:VAL:HG21	1:J:127:CYS:SG	2.50	0.52
1:J:116:MET:CE	1:J:118:ILE:HD11	2.39	0.52
1:I:50:VAL:CG2	1:I:127:CYS:SG	2.99	0.51
1:D:37:LEU:HD11	1:D:52:LEU:HD22	1.93	0.51
1:B:6:LEU:HD23	1:C:21:PRO:HB2	1.93	0.50
1:F:18:PRO:HG2	1:J:7:MET:CE	2.42	0.50
1:A:173:LYS:HE2	1:B:45:SER:O	2.11	0.50
1:F:172:SER:O	1:F:207[B]:ARG:HD3	2.12	0.49
1:I:156:LEU:HD13	1:I:198:VAL:HG23	1.93	0.49
1:B:106:ILE:HB	1:C:148:VAL:HG11	1.94	0.49
1:A:50:VAL:CG2	1:A:127:CYS:SG	3.01	0.49
1:A:25:LYS:NZ	6:E:400:NAG:H62	2.27	0.49
1:E:190:CYS:SG	1:E:191:CYS:N	2.85	0.49
1:G:147:TRP:O	2:G:300:AN4:N1	2.46	0.48
1:B:105:GLN:HA	1:B:105:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:TYR:HB3	3:F:300:AN5:C14	2.30	0.48
1:C:16:ARG:O	1:C:16:ARG:HG2	2.14	0.48
1:H:151:GLY:HA2	1:H:196:ILE:HD12	1.96	0.48
1:D:89:ASP:OD2	1:D:148:VAL:HG22	2.14	0.47
1:D:43:ALA:HA	1:D:50:VAL:HG22	1.96	0.47
1:I:13:LEU:O	1:I:17:SER:OG	2.30	0.47
1:C:7:MET:HG3	1:D:21:PRO:HG3	1.97	0.47
1:G:-2:ASP:O	1:G:1:HIS:HB2	2.14	0.47
1:F:97:ARG:HB2	1:F:124:SER:HB2	1.97	0.47
1:J:3:GLN:O	1:J:7:MET:HE2	2.14	0.47
1:E:185:VAL:HG22	1:E:196:ILE:HD13	1.96	0.47
1:J:91:THR:HG22	1:J:92:ALA:O	2.15	0.47
1:G:143:LYS:HE3	1:G:186:GLN:HE22	1.80	0.47
1:J:9:LEU:HA	1:J:72:TYR:CE1	2.50	0.47
1:C:133:ASP:O	1:C:208:ARG:NH2	2.48	0.46
1:F:17:SER:HB3	1:F:18:PRO:HD2	1.98	0.46
1:J:156:LEU:O	1:J:183:ARG:HD2	2.16	0.46
1:A:79:ARG:HD3	1:B:149:TYR:CE1	2.50	0.46
1:G:7:MET:HE3	1:H:18:PRO:HG2	1.97	0.45
1:F:50:VAL:CG2	1:F:127:CYS:SG	3.04	0.45
1:B:190:CYS:SG	2:B:300:AN4:H22C	2.56	0.45
1:E:156:LEU:HD13	1:E:198:VAL:HG23	1.99	0.45
1:A:59:ARG:NH1	1:A:159:ASP:OD1	2.50	0.45
1:F:135:GLU:O	1:F:205:ARG:NH2	2.48	0.45
1:D:51:ASP:HA	1:D:123:LEU:O	2.17	0.45
1:E:110:THR:HG22	1:E:111:HIS:N	2.31	0.45
1:A:99:VAL:HG13	1:A:121:GLN:HB3	1.99	0.44
1:B:169:TYR:CZ	1:B:171:SER:HB2	2.53	0.44
1:A:50:VAL:HG23	1:A:127:CYS:HB3	1.99	0.44
1:H:52:LEU:HG	1:H:125:PHE:HE2	1.83	0.44
1:C:12:ASP:O	1:C:16:ARG:HD2	2.17	0.44
1:I:155:ASP:OD1	1:I:183:ARG:NH2	2.49	0.44
1:J:110:THR:HG22	1:J:111:HIS:N	2.33	0.44
1:I:184:GLN:NE2	1:I:199:ASN:HB2	2.33	0.43
1:G:12:ASP:OD1	1:G:72:TYR:OH	2.23	0.43
1:D:143:LYS:HE3	1:D:184:GLN:NE2	2.33	0.43
1:A:100:GLN:NE2	1:A:122:ARG:HD2	2.33	0.43
1:A:163:VAL:HG22	1:A:181:GLN:HG3	2.01	0.43
1:H:103:SER:HB3	1:H:120:ALA:HB3	2.01	0.43
1:J:147:TRP:CE3	2:J:300:AN4:H51C	2.53	0.43
1:I:106:ILE:HB	1:J:148:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ASP:OD1	1:C:196:ILE:HD13	2.20	0.42
1:F:51:ASP:OD2	1:F:122:ARG:NH1	2.52	0.42
1:A:51:ASP:HA	1:A:123:LEU:O	2.19	0.42
1:G:190:CYS:SG	2:G:300:AN4:H22C	2.59	0.42
1:I:70:ASN:H	1:I:70:ASN:HD22	1.66	0.42
1:A:6:LEU:HD22	1:B:24:THR:HG22	2.01	0.42
1:I:207:ARG:O	1:I:208:ARG:CB	2.67	0.42
1:B:38:GLN:HE21	4:C:300:PG4:H81	1.85	0.42
1:G:106:ILE:HB	1:H:148:VAL:HG11	2.01	0.42
1:B:-2:ASP:O	1:B:1:HIS:HB2	2.20	0.42
1:F:106:ILE:HG21	1:G:148:VAL:HG21	2.02	0.42
1:B:147:TRP:O	2:B:300:AN4:N1	2.53	0.41
1:B:50:VAL:HG23	1:B:127:CYS:HB3	2.01	0.41
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.61	0.41
1:I:52:LEU:HG	1:I:125:PHE:HE2	1.86	0.41
1:I:110:THR:HG22	1:I:111:HIS:N	2.35	0.41
1:B:52:LEU:O	1:B:122:ARG:HA	2.20	0.41
1:C:204:PHE:CD2	1:C:204:PHE:N	2.89	0.41
1:F:18:PRO:CG	1:J:7:MET:SD	3.01	0.41
1:D:156:LEU:HD12	1:D:197:ASP:HA	2.03	0.41
1:A:67:TRP:CE3	1:A:111:HIS:HA	2.56	0.41
1:F:99:VAL:HG13	1:F:121:GLN:HB3	2.03	0.41
1:B:2:SER:HA	1:B:5:ASN:HD22	1.87	0.40
1:G:32:THR:HA	1:G:157:LYS:O	2.20	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	213/227 (94%)	210 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	208/227 (92%)	201 (97%)	7 (3%)	0	100	100
1	C	206/227 (91%)	201 (98%)	5 (2%)	0	100	100
1	D	211/227 (93%)	207 (98%)	4 (2%)	0	100	100
1	E	212/227 (93%)	207 (98%)	5 (2%)	0	100	100
1	F	210/227 (92%)	204 (97%)	6 (3%)	0	100	100
1	G	206/227 (91%)	200 (97%)	6 (3%)	0	100	100
1	H	210/227 (92%)	208 (99%)	2 (1%)	0	100	100
1	I	210/227 (92%)	206 (98%)	4 (2%)	0	100	100
1	J	211/227 (93%)	206 (98%)	5 (2%)	0	100	100
All	All	2097/2270 (92%)	2050 (98%)	47 (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	196/205 (96%)	185 (94%)	11 (6%)	21	45
1	B	192/205 (94%)	185 (96%)	7 (4%)	35	64
1	C	191/205 (93%)	184 (96%)	7 (4%)	34	63
1	D	193/205 (94%)	186 (96%)	7 (4%)	35	64
1	E	195/205 (95%)	188 (96%)	7 (4%)	35	64
1	F	193/205 (94%)	187 (97%)	6 (3%)	40	69
1	G	191/205 (93%)	180 (94%)	11 (6%)	20	43
1	H	193/205 (94%)	184 (95%)	9 (5%)	26	54
1	I	193/205 (94%)	184 (95%)	9 (5%)	26	54
1	J	193/205 (94%)	182 (94%)	11 (6%)	20	44
All	All	1930/2050 (94%)	1845 (96%)	85 (4%)	28	56

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	ASP
1	A	7	MET
1	A	17	SER
1	A	46	SER
1	A	64	SER
1	A	105	GLN
1	A	122	ARG
1	A	135	GLU
1	A	157	LYS
1	A	189	SER
1	A	208	ARG
1	B	55	TYR
1	B	105	GLN
1	B	122	ARG
1	B	135	GLU
1	B	162	GLN
1	B	186	GLN
1	B	205	ARG
1	C	-2	ASP
1	C	55	TYR
1	C	59	ARG
1	C	99	VAL
1	C	122	ARG
1	C	157	LYS
1	C	193	GLU
1	D	8	ARG
1	D	17	SER
1	D	25	LYS
1	D	29	LEU
1	D	122	ARG
1	D	186	GLN
1	D	189	SER
1	E	-3	ASP
1	E	59	ARG
1	E	64	SER
1	E	105	GLN
1	E	116	MET
1	E	189	SER
1	E	208	ARG
1	F	2	SER
1	F	7	MET
1	F	8	ARG

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Mol	Chain	Res	Type
1	F	17	SER
1	F	97	ARG
1	F	122	ARG
1	G	-2	ASP
1	G	0	LEU
1	G	59	ARG
1	G	121	GLN
1	G	122	ARG
1	G	135	GLU
1	G	161	ASP
1	G	162	GLN
1	G	182	THR
1	G	189	SER
1	G	193	GLU
1	H	11	SER
1	H	116	MET
1	H	122	ARG
1	H	130	THR
1	H	136	GLU
1	H	157	LYS
1	H	162	GLN
1	H	182	THR
1	H	207	ARG
1	I	16	ARG
1	I	17	SER
1	I	33	LEU
1	I	64	SER
1	I	71	GLU
1	I	122	ARG
1	I	136	GLU
1	I	186	GLN
1	I	193	GLU
1	J	7	MET
1	J	17	SER
1	J	19	MET
1	J	64	SER
1	J	66	MET
1	J	71	GLU
1	J	105	GLN
1	J	116	MET
1	J	122	ARG
1	J	193	GLU

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Mol	Chain	Res	Type
1	J	196	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	184	GLN
1	A	199	ASN
1	B	15	ASN
1	B	70	ASN
1	B	105	GLN
1	B	186	GLN
1	B	199	ASN
1	C	121	GLN
1	D	63	ASN
1	D	184	GLN
1	D	199	ASN
1	E	63	ASN
1	E	105	GLN
1	E	184	GLN
1	E	199	ASN
1	F	3	GLN
1	F	63	ASN
1	F	70	ASN
1	F	184	GLN
1	F	199	ASN
1	G	15	ASN
1	G	105	GLN
1	H	15	ASN
1	H	121	GLN
1	I	105	GLN
1	I	199	ASN
1	J	63	ASN
1	J	105	GLN
1	J	199	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	F	400	1	14,14,15	0.49	0	17,19,21	1.15	1 (5%)
3	AN5	F	300	-	13,13,13	0.78	1 (7%)	15,15,15	2.02	4 (26%)
6	NAG	H	400	1	14,14,15	0.42	0	17,19,21	1.04	0
3	AN5	D	300	-	13,13,13	0.35	0	15,15,15	1.47	4 (26%)
3	AN5	I	300	-	13,13,13	0.80	0	15,15,15	0.81	1 (6%)
4	PG4	C	300	-	12,12,12	0.50	0	11,11,11	0.26	0
2	AN4	A	300[B]	-	13,13,13	0.92	1 (7%)	14,16,16	2.50	2 (14%)
3	AN5	A	301[A]	-	13,13,13	0.53	0	15,15,15	1.21	2 (13%)
2	AN4	J	300	-	13,13,13	1.20	1 (7%)	14,16,16	2.35	4 (28%)
6	NAG	E	400	1	14,14,15	0.56	0	17,19,21	1.17	2 (11%)
2	AN4	B	300	-	13,13,13	1.01	1 (7%)	14,16,16	2.84	4 (28%)
2	AN4	G	300	-	13,13,13	1.06	1 (7%)	14,16,16	2.91	2 (14%)
2	AN4	E	300	-	13,13,13	0.89	1 (7%)	14,16,16	2.67	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	400	1	-	2/6/23/26	0/1/1/1
3	AN5	F	300	-	-	6/9/9/9	0/1/1/1
6	NAG	H	400	1	-	0/6/23/26	0/1/1/1
3	AN5	D	300	-	-	7/9/9/9	0/1/1/1
3	AN5	I	300	-	-	7/9/9/9	0/1/1/1
4	PG4	C	300	-	-	4/10/10/10	-
2	AN4	A	300[B]	-	-	3/4/12/12	0/2/2/2
3	AN5	A	301[A]	-	-	5/9/9/9	0/1/1/1
2	AN4	J	300	-	-	3/4/12/12	0/2/2/2
6	NAG	E	400	1	-	0/6/23/26	0/1/1/1
2	AN4	B	300	-	-	3/4/12/12	0/2/2/2
2	AN4	G	300	-	-	3/4/12/12	0/2/2/2
2	AN4	E	300	-	-	0/4/12/12	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	300	AN4	C1-N1	-3.85	1.25	1.28
2	B	300	AN4	C1-N1	-3.37	1.25	1.28
2	G	300	AN4	C1-N1	-3.35	1.26	1.28
2	A	300[B]	AN4	C1-N1	-2.50	1.26	1.28
2	E	300	AN4	C1-N1	-2.36	1.26	1.28
3	F	300	AN5	C15-C16	2.09	1.52	1.49

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	300	AN4	C5-N1-C1	9.82	130.87	117.16
2	B	300	AN4	C5-N1-C1	9.18	129.97	117.16
2	E	300	AN4	C5-N1-C1	8.75	129.37	117.16
2	A	300[B]	AN4	C5-N1-C1	8.42	128.92	117.16
2	J	300	AN4	C5-N1-C1	6.78	126.62	117.16
3	F	300	AN5	C17-C16-C15	5.83	127.22	119.13
6	F	400	NAG	O5-C5-C6	3.52	112.72	107.20
6	E	400	NAG	O5-C5-C6	3.48	112.65	107.20
2	J	300	AN4	C2-C1-C70	3.04	122.90	120.29
3	F	300	AN5	O11-C16-C15	-2.89	116.65	120.74
2	E	300	AN4	C4-C5-N1	-2.75	105.23	113.34
3	A	301[A]	AN5	C17-C16-C15	2.70	122.88	119.13
2	J	300	AN4	C9-N2-C10	2.64	121.42	116.85
3	D	300	AN5	C13-N11-C14	2.61	121.37	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	300	AN4	C9-N2-C10	2.59	121.32	116.85
2	G	300	AN4	C9-N2-C10	2.55	121.26	116.85
3	F	300	AN5	O11-C16-C17	-2.48	116.14	120.38
2	B	300	AN4	C4-C5-N1	-2.44	106.13	113.34
3	D	300	AN5	O11-C16-C15	-2.43	117.30	120.74
2	B	300	AN4	C9-N2-C10	2.30	120.82	116.85
3	I	300	AN5	C13-N11-C14	2.25	120.75	116.85
6	E	400	NAG	C4-C3-C2	2.25	114.32	111.02
2	A	300[B]	AN4	C9-N2-C10	2.22	120.68	116.85
3	D	300	AN5	C15-C14-N11	-2.18	120.28	123.49
3	A	301[A]	AN5	C13-N11-C14	2.08	120.45	116.85
3	F	300	AN5	C18-C17-C16	-2.05	109.84	113.62
2	B	300	AN4	C7-C70-C10	2.02	119.92	117.63
3	D	300	AN5	C17-C16-C15	2.02	121.93	119.13
2	J	300	AN4	C10-C70-C1	-2.01	119.80	121.36

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	300	AN5	C11-C15-C16-C17
3	F	300	AN5	C11-C15-C16-O11
3	F	300	AN5	C14-C15-C16-C17
3	F	300	AN5	C14-C15-C16-O11
2	A	300[B]	AN4	N1-C1-C70-C7
2	A	300[B]	AN4	N1-C1-C70-C10
2	A	300[B]	AN4	C2-C1-C70-C7
3	A	301[A]	AN5	C11-C15-C16-C17
3	A	301[A]	AN5	C11-C15-C16-O11
3	A	301[A]	AN5	C14-C15-C16-C17
3	A	301[A]	AN5	C14-C15-C16-O11
2	J	300	AN4	N1-C1-C70-C7
2	J	300	AN4	N1-C1-C70-C10
2	J	300	AN4	C2-C1-C70-C7
2	B	300	AN4	N1-C1-C70-C7
2	B	300	AN4	N1-C1-C70-C10
2	B	300	AN4	C2-C1-C70-C7
2	G	300	AN4	N1-C1-C70-C7
2	G	300	AN4	N1-C1-C70-C10
2	G	300	AN4	C2-C1-C70-C7
6	F	400	NAG	C4-C5-C6-O6
3	D	300	AN5	O11-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	D	300	AN5	C15-C16-C17-C18
3	D	300	AN5	C16-C17-C18-C1
3	I	300	AN5	C18-C1-C10-N12
3	F	300	AN5	C16-C17-C18-C1
6	F	400	NAG	O5-C5-C6-O6
4	C	300	PG4	O3-C5-C6-O4
4	C	300	PG4	C1-C2-O2-C3
3	F	300	AN5	C10-C1-C18-C17
3	D	300	AN5	C11-C15-C16-O11
3	D	300	AN5	C14-C15-C16-O11
3	D	300	AN5	C11-C15-C16-C17
3	D	300	AN5	C14-C15-C16-C17
4	C	300	PG4	C8-C7-O4-C6
3	I	300	AN5	C11-C15-C16-O11
3	I	300	AN5	C14-C15-C16-O11
3	I	300	AN5	C11-C15-C16-C17
3	I	300	AN5	C14-C15-C16-C17
3	A	301[A]	AN5	C16-C17-C18-C1
3	I	300	AN5	C16-C17-C18-C1
4	C	300	PG4	O2-C3-C4-O3
3	I	300	AN5	C15-C16-C17-C18

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	300	AN5	3	0
4	C	300	PG4	1	0
2	A	300[B]	AN4	2	0
3	A	301[A]	AN5	1	0
2	J	300	AN4	4	0
6	E	400	NAG	1	0
2	B	300	AN4	2	0
2	G	300	AN4	2	0

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	213/227 (93%)	-0.17	4 (1%) 66 69	20, 32, 57, 81	0
1	B	211/227 (92%)	-0.06	5 (2%) 59 60	21, 35, 74, 100	0
1	C	209/227 (92%)	0.01	2 (0%) 82 83	24, 36, 70, 95	0
1	D	212/227 (93%)	0.17	5 (2%) 59 60	25, 41, 82, 111	0
1	E	214/227 (94%)	0.02	4 (1%) 66 69	25, 41, 69, 93	0
1	F	211/227 (92%)	-0.18	2 (0%) 84 85	20, 31, 54, 77	0
1	G	210/227 (92%)	0.00	3 (1%) 75 77	23, 38, 73, 101	0
1	H	212/227 (93%)	0.03	4 (1%) 66 69	26, 39, 67, 77	0
1	I	211/227 (92%)	-0.05	5 (2%) 59 60	23, 36, 74, 102	0
1	J	212/227 (93%)	-0.21	1 (0%) 91 92	22, 37, 62, 78	0
All	All	2115/2270 (93%)	-0.04	35 (1%) 70 72	20, 37, 70, 111	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	HIS	5.1
1	A	-4	ASP	4.5
1	H	18	PRO	3.9
1	A	-3	ASP	3.9
1	H	19	MET	3.7
1	C	0	LEU	3.6
1	D	16	ARG	3.6
1	H	208	ARG	3.3
1	E	19	MET	3.3
1	B	-3	ASP	3.1
1	F	208	ARG	3.1
1	J	16	ARG	2.8
1	B	1	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	16	ARG	2.7
1	I	208	ARG	2.7
1	G	-1	LYS	2.7
1	D	1	HIS	2.7
1	I	-1	LYS	2.7
1	H	17	SER	2.6
1	B	-1	LYS	2.6
1	F	19	MET	2.5
1	I	16	ARG	2.5
1	A	1	HIS	2.4
1	D	19	MET	2.4
1	E	18	PRO	2.3
1	G	0	LEU	2.3
1	A	19	MET	2.2
1	C	16	ARG	2.2
1	I	2	SER	2.1
1	D	-2	ASP	2.1
1	B	0	LEU	2.1
1	D	4	ALA	2.1
1	B	17	SER	2.1
1	G	-3	ASP	2.1
1	E	-5	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AN5	D	300	13/13	0.81	0.25	37,39,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	E	1209	1/1	0.83	0.10	45,45,45,45	0
6	NAG	E	400	14/15	0.83	0.39	37,43,45,46	0
6	NAG	F	400	14/15	0.88	0.29	35,40,43,44	0
4	PG4	C	300	13/13	0.88	0.16	67,69,70,70	0
3	AN5	F	300	13/13	0.89	0.19	28,32,33,33	0
2	AN4	J	300	12/12	0.89	0.21	47,48,48,48	0
3	AN5	I	300	13/13	0.90	0.23	33,36,38,38	0
3	AN5	A	301[A]	13/13	0.91	0.19	29,31,32,32	13
2	AN4	A	300[B]	12/12	0.92	0.17	27,28,29,29	12
6	NAG	H	400	14/15	0.94	0.14	27,28,29,29	0
2	AN4	G	300	12/12	0.94	0.21	45,45,46,46	0
2	AN4	B	300	12/12	0.95	0.21	44,45,45,45	0
2	AN4	E	300	12/12	0.95	0.21	55,55,56,56	0
5	MG	H	1209	1/1	0.96	0.14	60,60,60,60	0
5	MG	C	1209	1/1	0.96	0.14	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.