



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

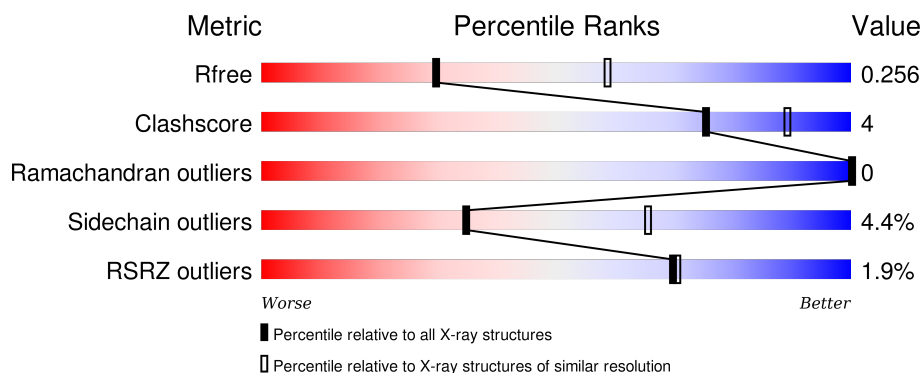
1 Overall quality at a glance

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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. 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>79%15%6%</div> </div>
1	B	227	<div> <div>2%</div> <div>80%11%7%</div> </div>
1	C	227	<div> <div>%</div> <div>82%9%8%</div> </div>
1	D	227	<div> <div>3%</div> <div>81%12%7%</div> </div>
1	E	227	<div> <div>2%</div> <div>85%9%6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	 83% 9% 7%
1	G	227	 80% 11% 7%
1	H	227	 82% 11% 7%
1	I	227	 79% 13% 7%
1	J	227	 79% 13% 7%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AN4	B	300	-	-	-	X
3	AN5	A	301	-	-	-	X
3	AN5	I	300	-	-	-	X

2 Entry composition

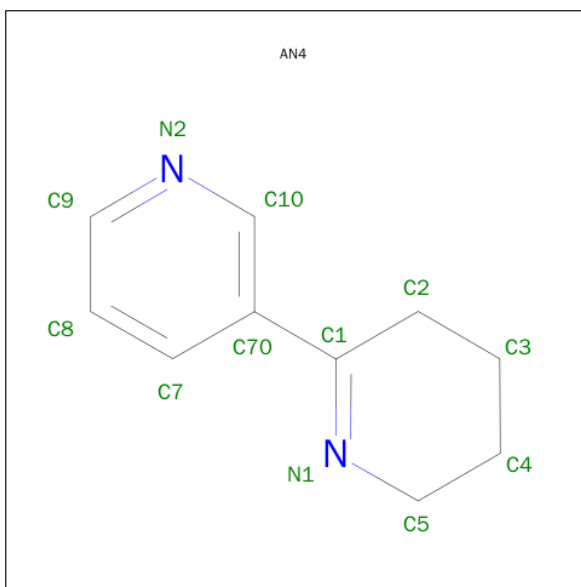
There are 7 unique types of molecules in this entry. The entry contains 17412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

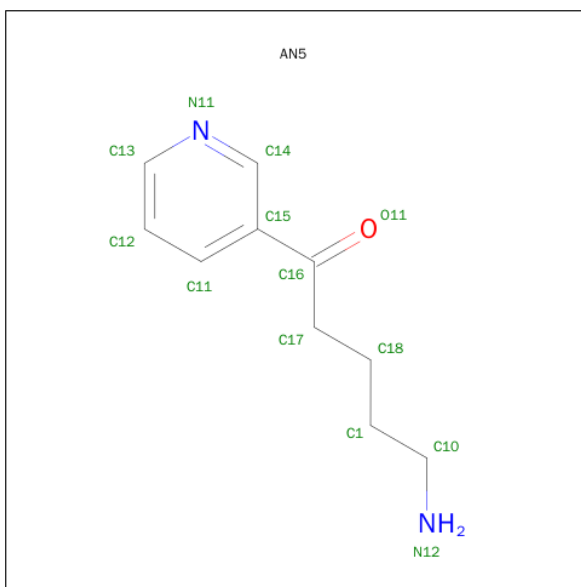
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	2	0
			1713	1079	283	342	9			
1	B	211	Total	C	N	O	S	0	1	0
			1690	1065	281	336	8			
1	C	209	Total	C	N	O	S	0	1	0
			1677	1058	279	332	8			
1	D	212	Total	C	N	O	S	0	1	0
			1697	1071	282	335	9			
1	E	214	Total	C	N	O	S	0	0	0
			1708	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).



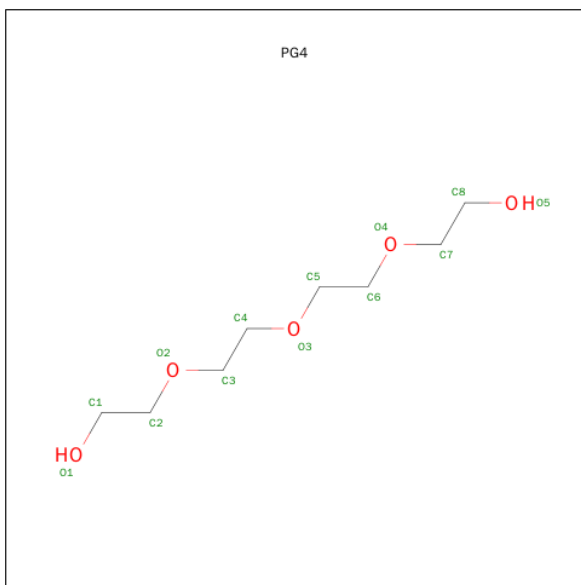
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			12	10	2		
2	B	1	Total	C	N	0	0
			12	10	2		
2	E	1	Total	C	N	0	0
			12	10	2		
2	G	1	Total	C	N	0	0
			12	10	2		
2	J	1	Total	C	N	0	0
			12	10	2		

- Molecule 3 is 5-AMINO-1-PYRIDIN-3-YLPENTAN-1-ONE (three-letter code: AN5) (formula: C₁₀H₁₄N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			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).

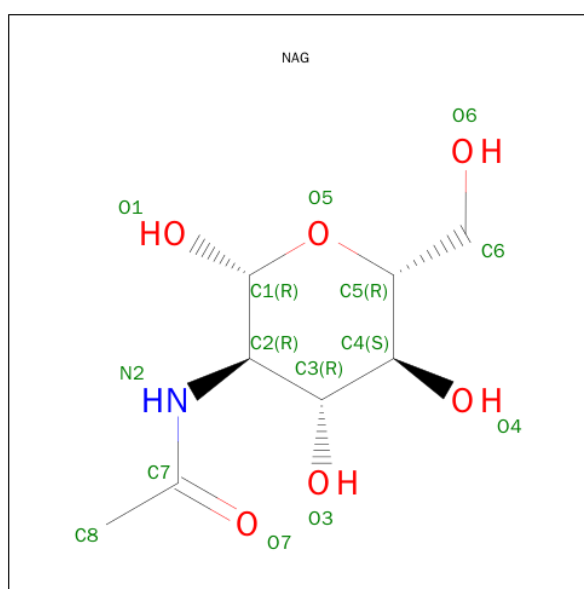


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	8	5		

- 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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (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		

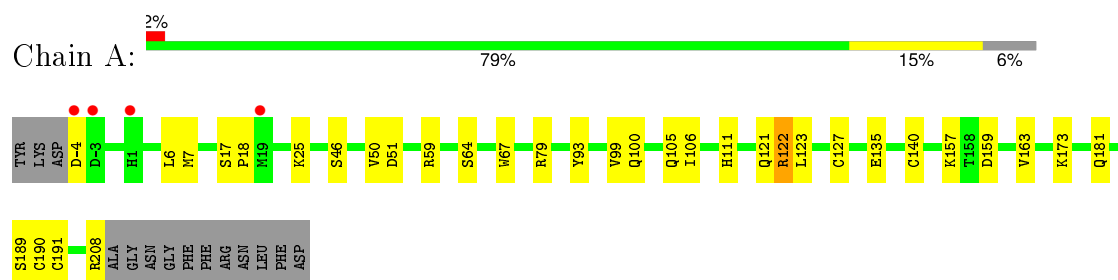
- Molecule 7 is water.

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

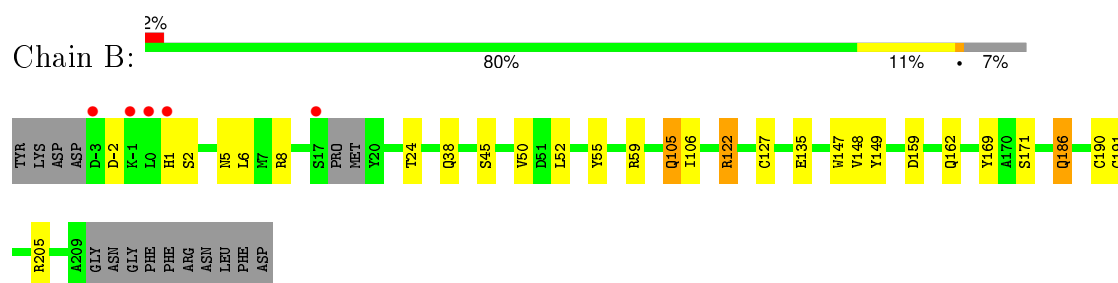
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

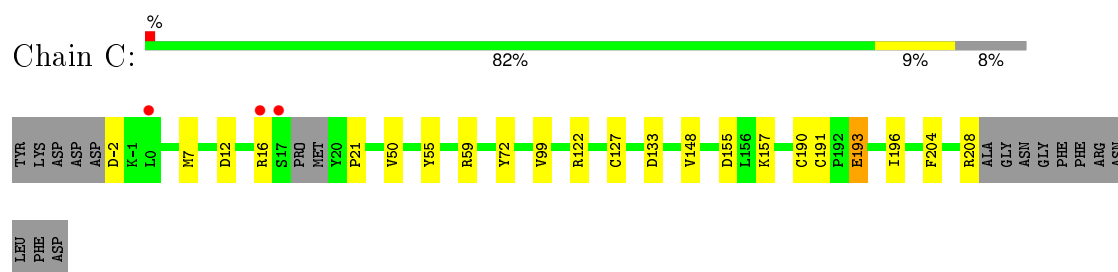
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



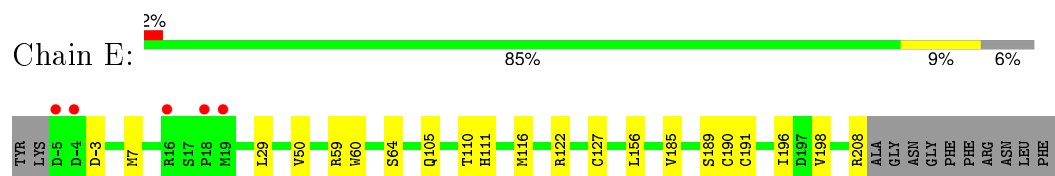
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



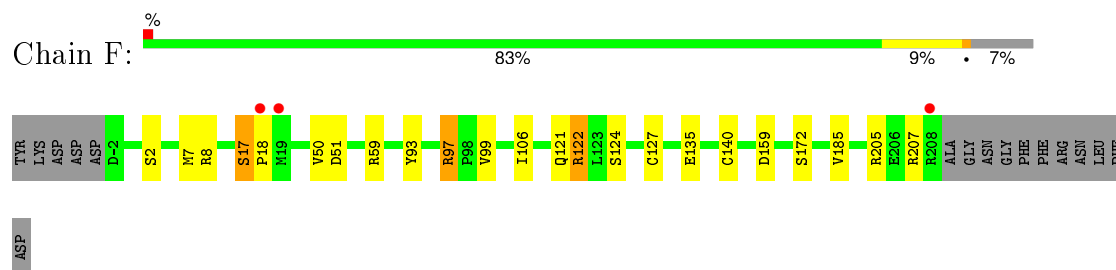
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



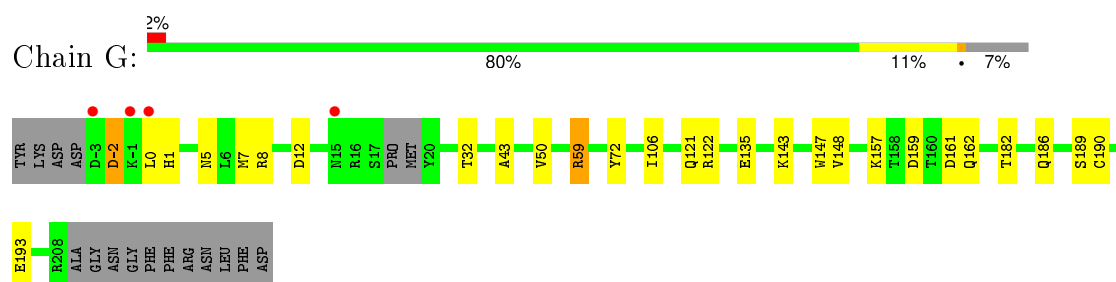
● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



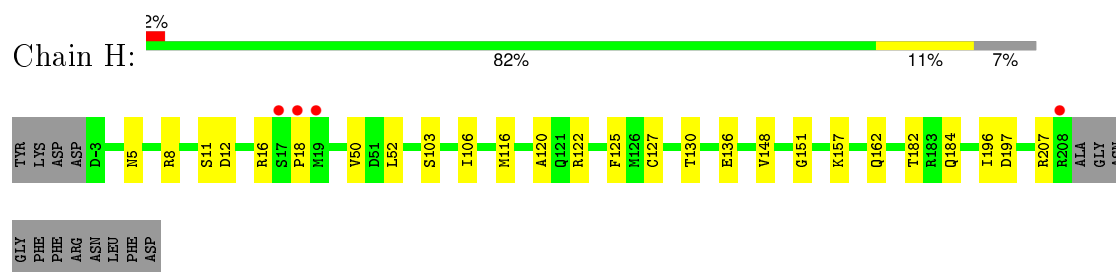
● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



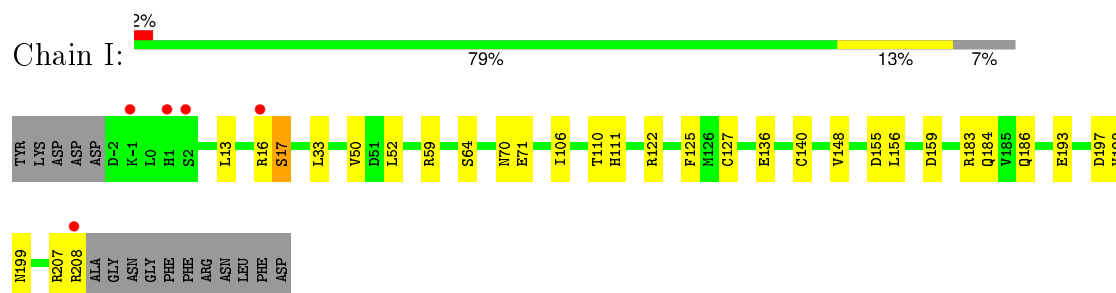
● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



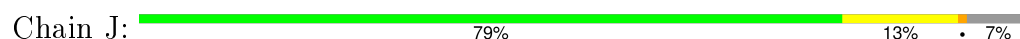
● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

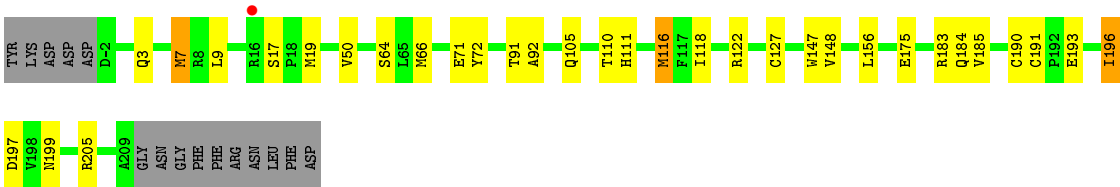


● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR





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 (3.11%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 72926 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	8	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	8	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

Continued on next page...

Continued from previous page...

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	16421	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: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: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:J:190:CYS:SG	1:J:191:CYS:N	2.75	0.60
1:C:191:CYS:HB3	1:C:193:GLU:OE2	2.01	0.60
1:D:29:LEU:HD11	1:D:62:LEU:CD2	2.32	0.60

Continued on next page...

Continued from previous page...

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: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:HA	1:B:105:GLN:HE21	1.67	0.58
1:D:8:ARG:HG3	1:D:8:ARG:HH11	1.70	0.57
1:A:190:CYS:SG	1:A:191:CYS:N	2.78	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:J:50:VAL:HG21	1:J:127:CYS:SG	2.50	0.52
1:I:59:ARG:NH2	1:I:159:ASP:OD2	2.42	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:F:93:TYR:HB3	3:F:300:AN5:C14	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLN:HA	1:B:105:GLN:NE2	2.29	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:J:3:GLN:O	1:J:7:MET:HE2	2.14	0.47
1:F:97:ARG:HB2	1:F:124:SER:HB2	1.97	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:J:9:LEU:HA	1:J:72:TYR:CE1	2.50	0.47
1:G:143:LYS:HE3	1:G:186:GLN:HE22	1.80	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:J:110:THR:HG22	1:J:111:HIS:N	2.33	0.44
1:I:155:ASP:OD1	1:I:183:ARG:NH2	2.49	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:163:VAL:HG22	1:A:181:GLN:HG3	2.01	0.43
1:A:100:GLN:NE2	1:A:122:ARG:HD2	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ASP:OD2	1:F:122:ARG:NH1	2.52	0.42
1:C:155:ASP:OD1	1:C:196:ILE:HD13	2.20	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:51:ASP:HA	1:A:123:LEU:O	2.19	0.42
1:I:207:ARG:O	1:I:208:ARG:CB	2.67	0.42
1:A:6:LEU:HD22	1:B:24:THR:HG22	2.01	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:F:106:ILE:HG21	1:G:148:VAL:HG21	2.02	0.42
1:B:-2:ASP:O	1:B:1:HIS:HB2	2.20	0.42
1:B:147:TRP:O	2:B:300:AN4:N1	2.53	0.41
1:I:52:LEU:HG	1:I:125:PHE:HE2	1.86	0.41
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.61	0.41
1:B:50:VAL:HG23	1:B:127:CYS:HB3	2.01	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:F:18:PRO:CG	1:J:7:MET:SD	3.01	0.41
1:C:204:PHE:CD2	1:C:204:PHE:N	2.89	0.41
1:D:156:LEU:HD12	1:D:197:ASP:HA	2.03	0.41
1:F:99:VAL:HG13	1:F:121:GLN:HB3	2.03	0.41
1:A:67:TRP:CE3	1:A:111:HIS:HA	2.56	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

Continued on next page...

Continued from previous page...

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%)	26	54
1	B	192/205 (94%)	185 (96%)	7 (4%)	42	73
1	C	191/205 (93%)	184 (96%)	7 (4%)	41	72
1	D	193/205 (94%)	186 (96%)	7 (4%)	42	73
1	E	195/205 (95%)	188 (96%)	7 (4%)	42	73
1	F	193/205 (94%)	187 (97%)	6 (3%)	47	78
1	G	191/205 (93%)	180 (94%)	11 (6%)	25	52
1	H	193/205 (94%)	184 (95%)	9 (5%)	32	63
1	I	193/205 (94%)	184 (95%)	9 (5%)	32	63
1	J	193/205 (94%)	182 (94%)	11 (6%)	25	53
All	All	1930/2050 (94%)	1845 (96%)	85 (4%)	35	65

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 carbohydrates 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	$\# Z > 2$
2	AN4	A	300	3	12,13,13	0.58	0	12,16,16	1.56	2 (16%)
3	AN5	A	301	2	13,13,13	0.51	0	15,15,15	1.12	1 (6%)
2	AN4	B	300	-	12,13,13	0.39	0	12,16,16	1.64	4 (33%)
4	PG4	C	300	-	12,12,12	0.51	0	11,11,11	0.24	0
3	AN5	D	300	-	13,13,13	0.35	0	15,15,15	1.40	3 (20%)
2	AN4	E	300	-	12,13,13	0.60	0	12,16,16	1.40	2 (16%)
6	NAG	E	400	1	14,14,15	0.56	0	15,19,21	1.08	2 (13%)
3	AN5	F	300	-	13,13,13	0.75	0	15,15,15	1.84	3 (20%)
6	NAG	F	400	1	14,14,15	0.47	0	15,19,21	0.97	1 (6%)
2	AN4	G	300	-	12,13,13	0.49	0	12,16,16	1.54	2 (16%)
6	NAG	H	400	1	14,14,15	0.41	0	15,19,21	0.90	0
3	AN5	I	300	-	13,13,13	0.77	0	15,15,15	0.76	1 (6%)
2	AN4	J	300	-	12,13,13	0.54	0	12,16,16	1.66	2 (16%)

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	AN4	A	300	3	-	0/4/12/12	0/2/2/2
3	AN5	A	301	2	-	0/9/9/9	0/1/1/1
2	AN4	B	300	-	-	0/4/12/12	0/2/2/2
4	PG4	C	300	-	-	0/10/10/10	0/0/0/0
3	AN5	D	300	-	-	0/9/9/9	0/1/1/1
2	AN4	E	300	-	-	0/4/12/12	0/2/2/2
6	NAG	E	400	1	-	0/6/23/26	0/1/1/1
3	AN5	F	300	-	-	0/9/9/9	0/1/1/1
6	NAG	F	400	1	-	0/6/23/26	0/1/1/1
2	AN4	G	300	-	-	0/4/12/12	0/2/2/2
6	NAG	H	400	1	-	0/6/23/26	0/1/1/1
3	AN5	I	300	-	-	0/9/9/9	0/1/1/1
2	AN4	J	300	-	-	0/4/12/12	0/2/2/2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	300	AN4	C4-C5-N1	-2.68	105.23	113.66
3	F	300	AN5	O11-C16-C15	-2.51	116.65	120.71
2	B	300	AN4	C4-C5-N1	-2.40	106.13	113.66
3	D	300	AN5	C15-C14-N11	-2.25	120.28	123.52
6	E	400	NAG	C3-C2-N2	-2.24	105.20	110.56
3	F	300	AN5	O11-C16-C17	-2.19	116.14	120.28
3	D	300	AN5	O11-C16-C15	-2.11	117.30	120.71
2	B	300	AN4	C70-C10-N2	-2.02	120.61	123.52
2	A	300	AN4	C9-N2-C10	2.08	120.68	116.84
3	I	300	AN5	C13-N11-C14	2.12	120.75	116.84
2	B	300	AN4	C9-N2-C10	2.16	120.82	116.84
2	G	300	AN4	C9-N2-C10	2.40	121.26	116.84
3	A	301	AN5	C17-C16-C15	2.42	122.88	119.23
2	E	300	AN4	C9-N2-C10	2.43	121.32	116.84
6	E	400	NAG	O5-C5-C6	2.45	112.65	107.35
3	D	300	AN5	C13-N11-C14	2.46	121.37	116.84
6	F	400	NAG	O5-C5-C6	2.48	112.72	107.35
2	J	300	AN4	C9-N2-C10	2.49	121.42	116.84
2	B	300	AN4	C70-C1-N1	2.54	121.17	118.02
2	G	300	AN4	C70-C1-N1	3.15	121.93	118.02
2	J	300	AN4	C70-C1-N1	3.93	122.90	118.02
2	A	300	AN4	C70-C1-N1	3.95	122.92	118.02
3	F	300	AN5	C17-C16-C15	5.31	127.22	119.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/227 (93%)	-0.14	4 (1%) 70 70	20, 32, 57, 81	0
1	B	211/227 (92%)	-0.03	5 (2%) 62 62	21, 35, 74, 100	0
1	C	209/227 (92%)	0.05	3 (1%) 78 77	24, 36, 70, 95	0
1	D	212/227 (93%)	0.21	6 (2%) 56 57	25, 41, 82, 111	0
1	E	214/227 (94%)	0.06	5 (2%) 64 64	25, 41, 69, 93	0
1	F	211/227 (92%)	-0.15	3 (1%) 78 77	20, 31, 54, 77	0
1	G	210/227 (92%)	0.04	4 (1%) 70 70	23, 38, 73, 101	0
1	H	212/227 (93%)	0.07	4 (1%) 70 70	26, 39, 67, 77	0
1	I	211/227 (92%)	-0.01	5 (2%) 62 62	23, 36, 74, 102	0
1	J	212/227 (93%)	-0.17	1 (0%) 91 93	22, 37, 62, 78	0
All	All	2115/2270 (93%)	-0.01	40 (1%) 70 70	20, 37, 70, 111	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	HIS	5.1
1	A	-4	ASP	4.7
1	A	-3	ASP	4.0
1	H	18	PRO	4.0
1	H	19	MET	3.8
1	D	16	ARG	3.7
1	C	0	LEU	3.7
1	E	19	MET	3.4
1	H	208	ARG	3.3
1	B	-3	ASP	3.3
1	F	208	ARG	3.1
1	J	16	ARG	2.9
1	B	1	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	16	ARG	2.8
1	G	-1	LYS	2.8
1	I	208	ARG	2.8
1	D	1	HIS	2.8
1	I	-1	LYS	2.7
1	B	-1	LYS	2.7
1	H	17	SER	2.7
1	F	19	MET	2.6
1	I	16	ARG	2.6
1	A	1	HIS	2.5
1	D	19	MET	2.5
1	E	18	PRO	2.4
1	G	0	LEU	2.3
1	A	19	MET	2.3
1	C	16	ARG	2.2
1	D	-2	ASP	2.2
1	I	2	SER	2.2
1	G	-3	ASP	2.2
1	D	4	ALA	2.1
1	E	-5	ASP	2.1
1	B	0	LEU	2.1
1	B	17	SER	2.1
1	D	136	GLU	2.1
1	G	15	ASN	2.0
1	C	17	SER	2.0
1	E	-4	ASP	2.0
1	F	18	PRO	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	AN5	A	301	13/13	0.91	0.19	2.81	29,31,32,32	13
2	AN4	B	300	12/12	0.95	0.21	2.67	44,45,45,45	0
3	AN5	I	300	13/13	0.90	0.23	2.03	33,36,38,38	0
2	AN4	A	300	12/12	0.93	0.17	1.70	27,28,29,29	12
2	AN4	G	300	12/12	0.94	0.21	1.67	45,45,46,46	0
2	AN4	J	300	12/12	0.89	0.21	1.26	47,48,48,48	0
3	AN5	D	300	13/13	0.81	0.25	1.22	37,39,39,41	0
3	AN5	F	300	13/13	0.89	0.19	0.92	28,32,33,33	0
2	AN4	E	300	12/12	0.95	0.21	0.36	55,55,56,56	0
4	PG4	C	300	13/13	0.88	0.16	-0.41	67,69,70,70	0
6	NAG	H	400	14/15	0.94	0.14	-0.63	27,28,29,29	0
5	MG	H	1209	1/1	0.96	0.14	-	60,60,60,60	0
6	NAG	F	400	14/15	0.88	0.29	-	35,40,43,44	0
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
5	MG	C	1209	1/1	0.96	0.14	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.