



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:59 PM GMT

PDB ID : 4B5D
Title : Capitella teleta AChBP in complex with psychonidine (3-((2(S)- Azetidinyloxy)-5-((1S,2R)-2-(2-hydroxyethyl)cyclopropyl)pyridine)
Authors : Nys, M.; Ulens, C.
Deposited on : 2012-08-03
Resolution : 2.19 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

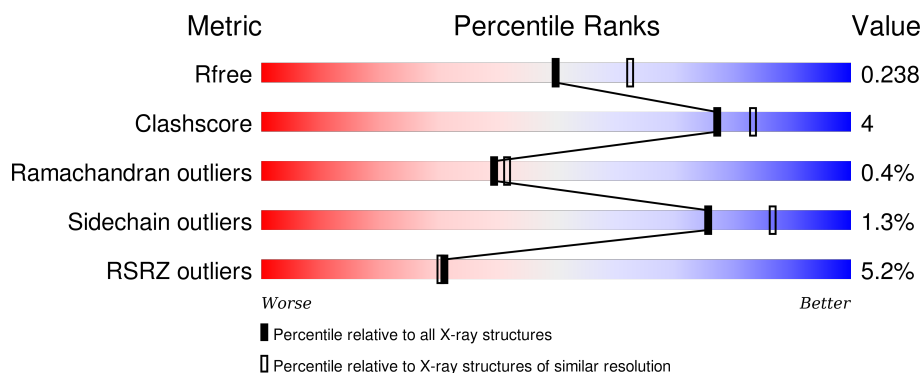
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	230	<div> <div>3%</div> <div>83% 9% 8%</div> </div>
1	B	230	<div> <div>4%</div> <div>83% 8% 8%</div> </div>
1	C	230	<div> <div>10%</div> <div>84% 8% 8%</div> </div>
1	D	230	<div> <div>4%</div> <div>80% 11% 8%</div> </div>
1	E	230	<div> <div>3%</div> <div>82% 10% 8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8938 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.

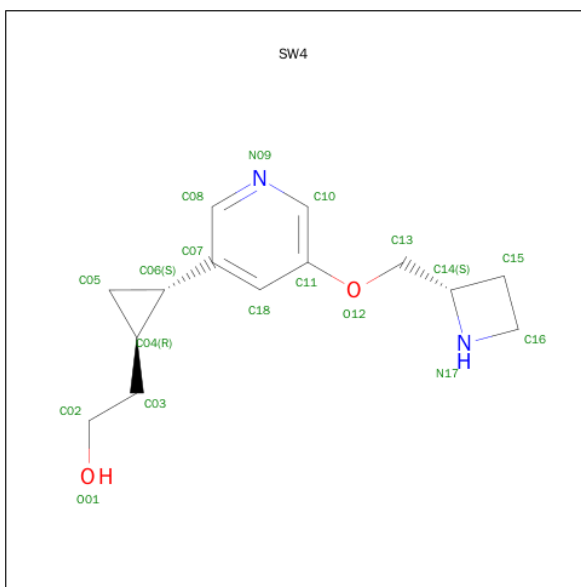
- Molecule 1 is a protein called CAPITELLA TELETA ACHBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1702	1098	272	323	9			
1	B	211	Total	C	N	O	S	0	0	0
			1702	1098	272	323	9			
1	C	211	Total	C	N	O	S	0	0	0
			1702	1098	272	323	9			
1	D	211	Total	C	N	O	S	0	0	0
			1702	1098	272	323	9			
1	E	211	Total	C	N	O	S	0	0	0
			1702	1098	272	323	9			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-[(1R,2S)-2-[5-[(2S)-AZETIDIN-2-YL]METHOXY]PYRIDIN-3-YL]CYCLOPROPYL]ETHANOL (three-letter code: SW4) (formula: C₁₄H₂₀N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	14	2	2		
3	B	1	Total	C	N	O	0	0
			18	14	2	2		
3	C	1	Total	C	N	O	0	0
			18	14	2	2		
3	D	1	Total	C	N	O	0	0
			18	14	2	2		
3	E	1	Total	C	N	O	0	0
			18	14	2	2		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

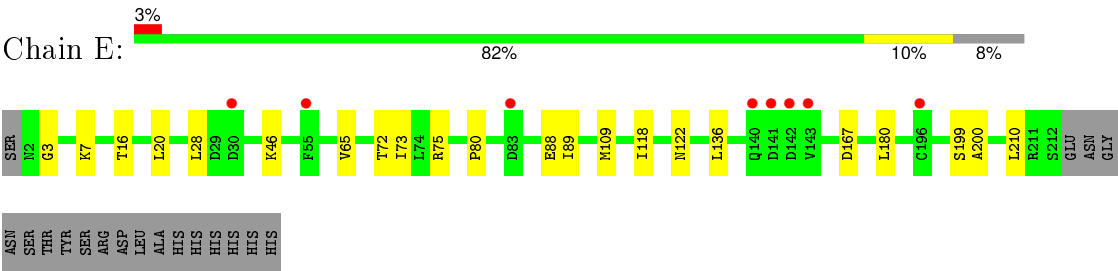
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	60	Total	O	0	0
			60	60		
5	C	30	Total	O	0	0
			30	30		
5	D	28	Total	O	0	0
			28	28		
5	E	42	Total	O	0	0
			42	42		

• Molecule 1: CAPITELLA TELETA ACHBP



● Molecule 1: CAPITELLA TELETA ACHBP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.36Å 114.28Å 135.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.43 – 2.19 47.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.43-2.19) 97.9 (47.43-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.191 , 0.242 0.188 , 0.238	Depositor DCC
R_{free} test set	3183 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 63986 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8938	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SW4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/1740	0.57	0/2361
1	B	0.41	0/1740	0.54	0/2361
1	C	0.36	0/1740	0.50	0/2361
1	D	0.38	0/1740	0.50	0/2361
1	E	0.41	0/1740	0.53	0/2361
All	All	0.40	0/8700	0.53	0/11805

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1702	0	1679	14	0
1	B	1702	0	1679	15	0
1	C	1702	0	1679	10	0
1	D	1702	0	1679	16	0
1	E	1702	0	1679	15	0
2	A	28	0	25	0	0
2	E	28	0	25	0	0
3	A	18	0	19	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	19	3	0
3	C	18	0	19	1	0
3	D	18	0	19	1	0
3	E	18	0	19	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	80	0	0	3	1
5	B	60	0	0	2	1
5	C	30	0	0	0	0
5	D	28	0	0	0	0
5	E	42	0	0	2	0
All	All	8938	0	8579	63	1

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 (63) 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:D:184:GLU:HB3	1:D:209:ALA:HB3	1.66	0.75
1:B:196:CYS:SG	5:B:2057:HOH:O	2.48	0.71
1:A:196:CYS:SG	5:A:2075:HOH:O	2.49	0.69
1:D:5:MET:HG3	1:D:81:PRO:HB2	1.79	0.65
3:D:1213:SW4:H051	1:E:118:ILE:HG13	1.82	0.61
3:C:1213:SW4:H051	1:D:118:ILE:HG13	1.84	0.59
1:A:202:VAL:HG12	1:A:204:MET:CE	2.33	0.59
1:B:10:ARG:NH2	1:B:88:GLU:OE1	2.38	0.57
1:A:72:THR:OG1	1:A:75:ARG:NH1	2.38	0.56
1:E:65:VAL:HG21	1:E:109:MET:HE2	1.88	0.56
1:D:24:GLY:HA2	1:E:88:GLU:OE2	2.07	0.54
1:A:202:VAL:HG12	1:A:204:MET:HE3	1.89	0.53
1:B:66:LYS:NZ	1:B:174:ASP:OD2	2.40	0.53
1:A:4:LEU:HA	5:A:2003:HOH:O	2.08	0.52
5:B:2038:HOH:O	1:C:86:LYS:NZ	2.43	0.52
1:B:27:PHE:O	1:C:3:GLY:HA3	2.10	0.52
1:E:28:LEU:HG	1:E:73:ILE:HG12	1.93	0.51
1:D:199:SER:OG	1:D:200:ALA:N	2.43	0.51
1:D:119:VAL:HG22	1:D:125:VAL:HG22	1.93	0.51
5:A:2003:HOH:O	1:E:20:LEU:HD13	2.10	0.50
1:B:109:MET:HE2	1:B:131:ALA:HB1	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:HE3	1:B:133:LEU:HG	1.93	0.49
1:E:89:ILE:HB	5:E:2022:HOH:O	2.13	0.48
1:E:180:LEU:HD13	1:E:210:LEU:HD13	1.96	0.48
3:B:1213:SW4:H051	1:C:118:ILE:HG13	1.94	0.48
1:D:89:ILE:HD12	1:D:119:VAL:HG21	1.96	0.47
1:C:25:LEU:HD11	1:C:159:GLU:HB3	1.95	0.47
1:B:66:LYS:HG2	1:B:128:ILE:HG23	1.97	0.46
3:A:1213:SW4:H051	1:B:118:ILE:HG13	1.97	0.46
1:B:51:ARG:HH12	1:B:136:LEU:HD11	1.81	0.46
1:A:174:ASP:OD1	1:A:174:ASP:N	2.47	0.45
1:E:199:SER:OG	1:E:200:ALA:N	2.48	0.45
1:D:20:LEU:HB3	1:E:7:LYS:HB3	1.98	0.45
1:B:174:ASP:N	1:B:174:ASP:OD1	2.50	0.45
1:C:199:SER:OG	1:C:200:ALA:N	2.45	0.45
1:A:28:LEU:HG	1:A:73:ILE:HG12	1.99	0.45
1:B:6:ALA:HB2	1:B:84:PHE:CZ	2.52	0.44
1:D:27:PHE:O	1:E:3:GLY:HA3	2.17	0.44
1:D:85:GLN:CD	1:D:85:GLN:H	2.21	0.44
1:E:136:LEU:HD23	1:E:136:LEU:HA	1.89	0.44
1:D:80:PRO:HA	1:D:81:PRO:HA	1.69	0.44
1:A:190:GLN:OE1	1:A:205:LYS:HD2	2.17	0.43
1:B:51:ARG:NH1	1:B:136:LEU:HD11	2.33	0.43
1:C:28:LEU:HD13	1:D:4:LEU:HD13	2.01	0.43
1:A:109:MET:HB2	1:A:109:MET:HE2	1.87	0.43
1:E:80:PRO:HG3	5:E:2020:HOH:O	2.18	0.43
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.91	0.43
1:A:119:VAL:HG22	1:A:125:VAL:HG22	2.01	0.43
1:B:197:CYS:SG	3:B:1213:SW4:H132	2.59	0.42
1:A:65:VAL:HG21	1:A:109:MET:HE1	2.01	0.42
1:D:28:LEU:HG	1:D:73:ILE:HG12	2.01	0.42
1:A:26:PRO:O	1:A:72:THR:HG22	2.19	0.42
3:B:1213:SW4:H022	1:C:120:PHE:HZ	1.85	0.42
1:C:5:MET:HG3	1:C:81:PRO:HB2	2.02	0.42
1:E:75:ARG:HD2	1:E:122:ASN:O	2.20	0.42
1:E:16:THR:HG23	1:E:20:LEU:HD12	2.03	0.41
1:C:119:VAL:HG22	1:C:125:VAL:HG22	2.01	0.41
1:D:106:ASP:OD1	1:E:46:LYS:NZ	2.53	0.41
1:A:27:PHE:O	1:B:3:GLY:HA3	2.20	0.41
1:D:174:ASP:OD1	1:D:174:ASP:N	2.53	0.41
1:D:161:ASP:OD1	1:D:162:ILE:N	2.54	0.41
1:B:133:LEU:HD12	1:B:133:LEU:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:HD11	1:C:57:SER:OG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2067:HOH:O	5:B:2050:HOH:O[4_555]	2.19	0.01

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	209/230 (91%)	204 (98%)	4 (2%)	1 (0%)	34	35
1	B	209/230 (91%)	202 (97%)	7 (3%)	0	100	100
1	C	209/230 (91%)	201 (96%)	7 (3%)	1 (0%)	34	35
1	D	209/230 (91%)	198 (95%)	9 (4%)	2 (1%)	19	16
1	E	209/230 (91%)	202 (97%)	7 (3%)	0	100	100
All	All	1045/1150 (91%)	1007 (96%)	34 (3%)	4 (0%)	39	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	29	ASP
1	D	80	PRO
1	D	29	ASP
1	A	29	ASP

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	193/210 (92%)	191 (99%)	2 (1%)	82	91
1	B	193/210 (92%)	190 (98%)	3 (2%)	70	82
1	C	193/210 (92%)	191 (99%)	2 (1%)	82	91
1	D	193/210 (92%)	189 (98%)	4 (2%)	61	74
1	E	193/210 (92%)	191 (99%)	2 (1%)	82	91
All	All	965/1050 (92%)	952 (99%)	13 (1%)	76	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	212	SER
1	B	48	ILE
1	B	88	GLU
1	B	198	GLU
1	C	30	ASP
1	C	77	ASP
1	D	72	THR
1	D	88	GLU
1	D	145	SER
1	D	196	CYS
1	E	72	THR
1	E	167	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	177	GLN
1	D	188	GLN
1	D	190	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

4 carbohydrates 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	NAG	A	677	1,2	14,14,15	0.49	0	15,19,21	1.05	1 (6%)
2	NAG	A	678	2	14,14,15	0.53	0	15,19,21	0.72	0
2	NAG	E	677	1,2	14,14,15	0.60	0	15,19,21	0.87	0
2	NAG	E	678	2	14,14,15	0.64	0	15,19,21	0.74	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	NAG	A	677	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	678	2	-	0/6/23/26	0/1/1/1
2	NAG	E	677	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	678	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	677	NAG	C1-O5-C5	2.34	115.22	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	677	NAG	O7-C7-N2-C2
2	E	677	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SW4	A	1213	-	16,20,20	1.84	3 (18%)	19,27,27	2.12	6 (31%)
3	SW4	B	1213	-	16,20,20	2.06	3 (18%)	19,27,27	1.86	6 (31%)
4	NAG	B	677	1	14,14,15	0.53	0	15,19,21	1.37	1 (6%)
3	SW4	C	1213	-	16,20,20	2.00	3 (18%)	19,27,27	1.87	7 (36%)
4	NAG	C	677	1	14,14,15	0.51	0	15,19,21	1.73	3 (20%)
3	SW4	D	1213	-	16,20,20	2.06	3 (18%)	19,27,27	1.85	6 (31%)
4	NAG	D	677	1	14,14,15	0.48	0	15,19,21	1.51	2 (13%)
3	SW4	E	1213	-	16,20,20	2.02	3 (18%)	19,27,27	2.04	6 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SW4	A	1213	-	-	0/11/23/23	0/2/3/3
3	SW4	B	1213	-	-	0/11/23/23	0/2/3/3
4	NAG	B	677	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SW4	C	1213	-	-	0/11/23/23	0/2/3/3
4	NAG	C	677	1	-	0/6/23/26	0/1/1/1
3	SW4	D	1213	-	-	0/11/23/23	0/2/3/3
4	NAG	D	677	1	-	0/6/23/26	0/1/1/1
3	SW4	E	1213	-	-	0/11/23/23	0/2/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1213	SW4	C15-C16	-6.87	1.46	1.54
3	E	1213	SW4	C15-C16	-6.76	1.46	1.54
3	C	1213	SW4	C15-C16	-6.68	1.46	1.54
3	B	1213	SW4	C15-C16	-6.53	1.46	1.54
3	A	1213	SW4	C15-C16	-5.43	1.47	1.54
3	C	1213	SW4	C10-C11	2.11	1.41	1.38
3	E	1213	SW4	C10-C11	2.13	1.41	1.38
3	D	1213	SW4	O12-C11	2.23	1.43	1.37
3	D	1213	SW4	C10-C11	2.35	1.41	1.38
3	C	1213	SW4	O12-C11	2.38	1.43	1.37
3	B	1213	SW4	C10-C11	2.42	1.41	1.38
3	A	1213	SW4	O12-C11	2.48	1.43	1.37
3	E	1213	SW4	O12-C11	2.53	1.43	1.37
3	B	1213	SW4	O12-C11	2.72	1.44	1.37
3	A	1213	SW4	C10-C11	2.99	1.42	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1213	SW4	C18-C07-C06	-4.18	112.38	120.18
3	E	1213	SW4	C07-C08-N09	-3.88	118.02	124.27
3	A	1213	SW4	C07-C08-N09	-3.55	118.54	124.27
3	D	1213	SW4	C07-C08-N09	-3.51	118.61	124.27
3	C	1213	SW4	C07-C08-N09	-3.44	118.72	124.27
3	B	1213	SW4	C07-C08-N09	-3.42	118.74	124.27
4	C	677	NAG	C2-N2-C7	-2.98	119.21	123.04
3	A	1213	SW4	C11-C10-N09	-2.93	120.29	122.78
3	E	1213	SW4	C11-C10-N09	-2.87	120.34	122.78
3	E	1213	SW4	C18-C07-C06	-2.81	114.94	120.18
3	C	1213	SW4	C11-C10-N09	-2.64	120.53	122.78
3	B	1213	SW4	C18-C07-C06	-2.59	115.36	120.18
4	C	677	NAG	C4-C3-C2	-2.50	107.35	111.23
3	B	1213	SW4	C11-C10-N09	-2.40	120.74	122.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1213	SW4	C11-C10-N09	-2.30	120.83	122.78
3	D	1213	SW4	C18-C07-C06	-2.25	115.98	120.18
3	C	1213	SW4	C18-C07-C06	-2.25	115.99	120.18
3	C	1213	SW4	C15-C14-C13	-2.23	107.87	116.12
3	E	1213	SW4	C15-C14-C13	-2.22	107.87	116.12
4	D	677	NAG	C2-N2-C7	-2.16	120.26	123.04
3	D	1213	SW4	C15-C14-C13	-2.08	108.43	116.12
3	C	1213	SW4	O12-C13-C14	2.17	114.97	109.04
3	B	1213	SW4	O12-C13-C14	2.41	115.62	109.04
3	A	1213	SW4	C08-C07-C06	2.45	126.37	120.91
3	B	1213	SW4	C10-N09-C08	2.71	121.59	117.50
3	D	1213	SW4	C10-N09-C08	2.76	121.67	117.50
3	A	1213	SW4	C10-N09-C08	2.78	121.69	117.50
3	C	1213	SW4	C10-N09-C08	2.80	121.72	117.50
3	B	1213	SW4	C18-C07-C08	3.16	120.25	116.78
3	E	1213	SW4	C10-N09-C08	3.44	122.69	117.50
3	E	1213	SW4	C18-C07-C08	3.45	120.57	116.78
3	C	1213	SW4	C18-C07-C08	3.50	120.62	116.78
3	D	1213	SW4	C18-C07-C08	3.78	120.93	116.78
4	B	677	NAG	C1-O5-C5	3.86	117.15	112.25
3	A	1213	SW4	C18-C07-C08	4.06	121.23	116.78
4	D	677	NAG	C1-O5-C5	4.43	117.88	112.25
4	C	677	NAG	C1-O5-C5	5.11	118.73	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1213	SW4	1	0
3	B	1213	SW4	3	0
3	C	1213	SW4	1	0
3	D	1213	SW4	1	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	211/230 (91%)	0.31	6 (2%) 56 55	21, 37, 73, 101	0
1	B	211/230 (91%)	0.27	9 (4%) 39 38	23, 41, 78, 116	0
1	C	211/230 (91%)	0.53	22 (10%) 8 8	32, 55, 89, 118	0
1	D	211/230 (91%)	0.35	10 (4%) 35 34	34, 55, 91, 123	0
1	E	211/230 (91%)	0.24	8 (3%) 44 43	27, 45, 76, 104	0
All	All	1055/1150 (91%)	0.34	55 (5%) 31 30	21, 47, 85, 123	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	CYS	6.3
1	C	55	PHE	4.6
1	C	81	PRO	4.3
1	E	55	PHE	4.3
1	C	196	CYS	4.1
1	A	196	CYS	4.1
1	D	55	PHE	4.0
1	C	142	ASP	3.7
1	D	141	ASP	3.7
1	C	79	GLU	3.6
1	C	77	ASP	3.6
1	B	195	PRO	3.4
1	D	81	PRO	3.3
1	E	141	ASP	3.2
1	B	28	LEU	3.2
1	D	6	ALA	3.0
1	E	196	CYS	3.0
1	C	15	ASN	3.0
1	B	55	PHE	2.9
1	C	141	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	82	PHE	2.8
1	E	142	ASP	2.8
1	C	53	MET	2.8
1	C	140	GLN	2.8
1	A	81	PRO	2.7
1	E	143	VAL	2.7
1	E	30	ASP	2.6
1	C	4	LEU	2.6
1	D	82	PHE	2.6
1	C	184	GLU	2.5
1	E	140	GLN	2.5
1	D	5	MET	2.5
1	B	198	GLU	2.5
1	A	195	PRO	2.5
1	C	143	VAL	2.5
1	B	53	MET	2.4
1	D	196	CYS	2.4
1	C	28	LEU	2.4
1	C	80	PRO	2.3
1	D	53	MET	2.3
1	D	4	LEU	2.3
1	A	4	LEU	2.3
1	A	8	ARG	2.2
1	C	211	ARG	2.2
1	B	193	VAL	2.2
1	D	143	VAL	2.2
1	C	5	MET	2.1
1	B	4	LEU	2.1
1	C	83	ASP	2.1
1	C	158	ASP	2.1
1	B	142	ASP	2.1
1	E	83	ASP	2.1
1	C	183	LEU	2.1
1	C	19	GLN	2.1
1	A	80	PRO	2.0

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 [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
2	NAG	A	677	14/15	0.97	0.09	-1.62	44,57,66,82	0
2	NAG	E	677	14/15	0.96	0.13	-	45,68,84,86	0
2	NAG	A	678	14/15	0.78	0.16	-	100,112,116,117	0
2	NAG	E	678	14/15	0.67	0.26	-	105,124,132,134	0

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	SW4	E	1213	18/18	0.97	0.15	0.32	25,40,56,57	0
3	SW4	C	1213	18/18	0.95	0.14	-0.14	49,57,81,89	0
3	SW4	A	1213	18/18	0.97	0.14	-0.15	25,31,53,60	0
3	SW4	B	1213	18/18	0.95	0.13	-0.41	32,47,73,83	0
3	SW4	D	1213	18/18	0.94	0.12	-0.56	41,49,69,75	0
4	NAG	B	677	14/15	0.95	0.09	-1.16	38,53,61,64	0
4	NAG	D	677	14/15	0.90	0.12	-	64,78,83,83	0
4	NAG	C	677	14/15	0.89	0.12	-	70,77,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.