wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:12 PM GMT

PDB ID	:	4BTW
Title	:	Crystal structure of human vascular adhesion protein-1 in complex with pyridazinone inhibitors
Authors	:	Bligt-Linden, E.; Pihlavisto, M.; Szatmari, I.; Otwinowski, Z.; Smith, D.J.; Lazar, L.; Fulop, F.; Salminen, T.A.
Deposited on	:	2013-06-19
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

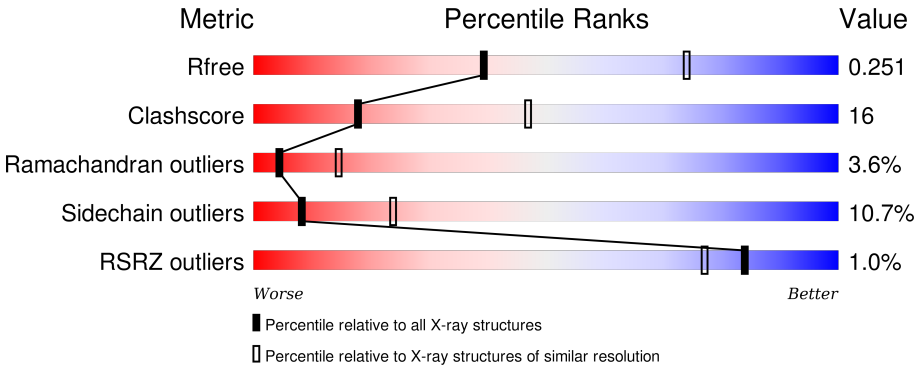
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	737	% 60% 30% 6% ·
1	B	737	% 59% 30% 6% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	1770	X	-	-	-
6	NAG	A	1771	X	-	-	-
6	NAG	B	1774	X	-	-	-
7	JW7	A	2000	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11573 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 MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5609	3599	970	1020	20			
1	B	705	Total	C	N	O	S	0	0	0
			5562	3571	959	1012	20			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

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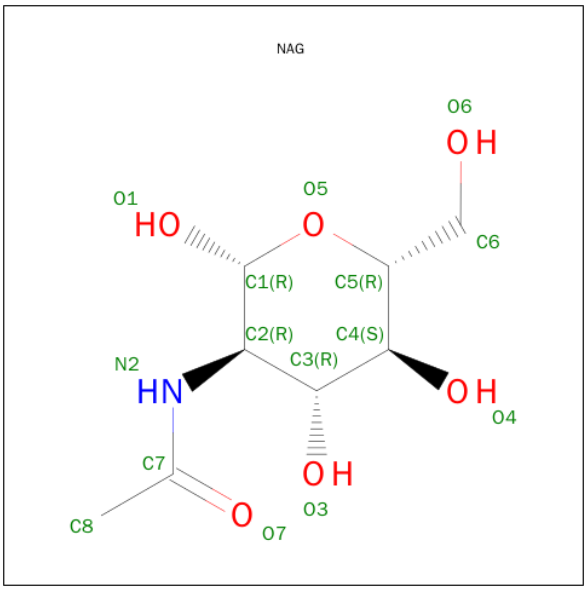
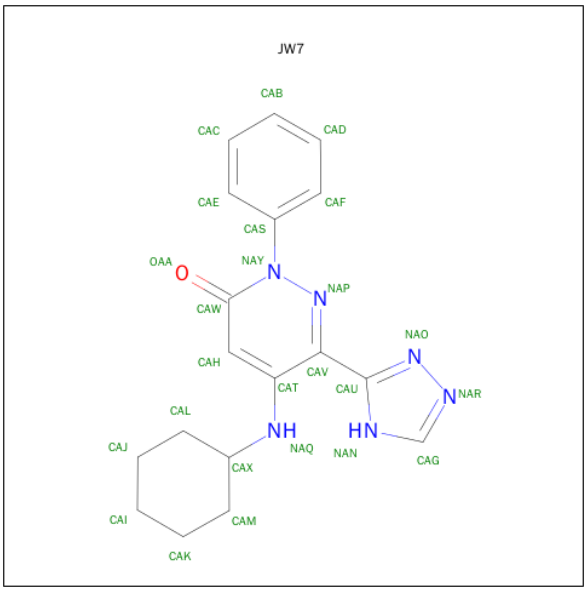
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is 5-(CYCLOHEXYLAMINO)-2-PHENYL-6-(1H-1,2,4-TRIAZOL-5-YL)-3(2H)-PYRIDAZINONE (three-letter code: JW7) (formula: $C_{18}H_{20}N_6O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 25 18 6 1	0	0
7	B	1	Total C N O 25 18 6 1	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	5	Total C N O 61 34 2 25	0	0

- Molecule 9 is water.

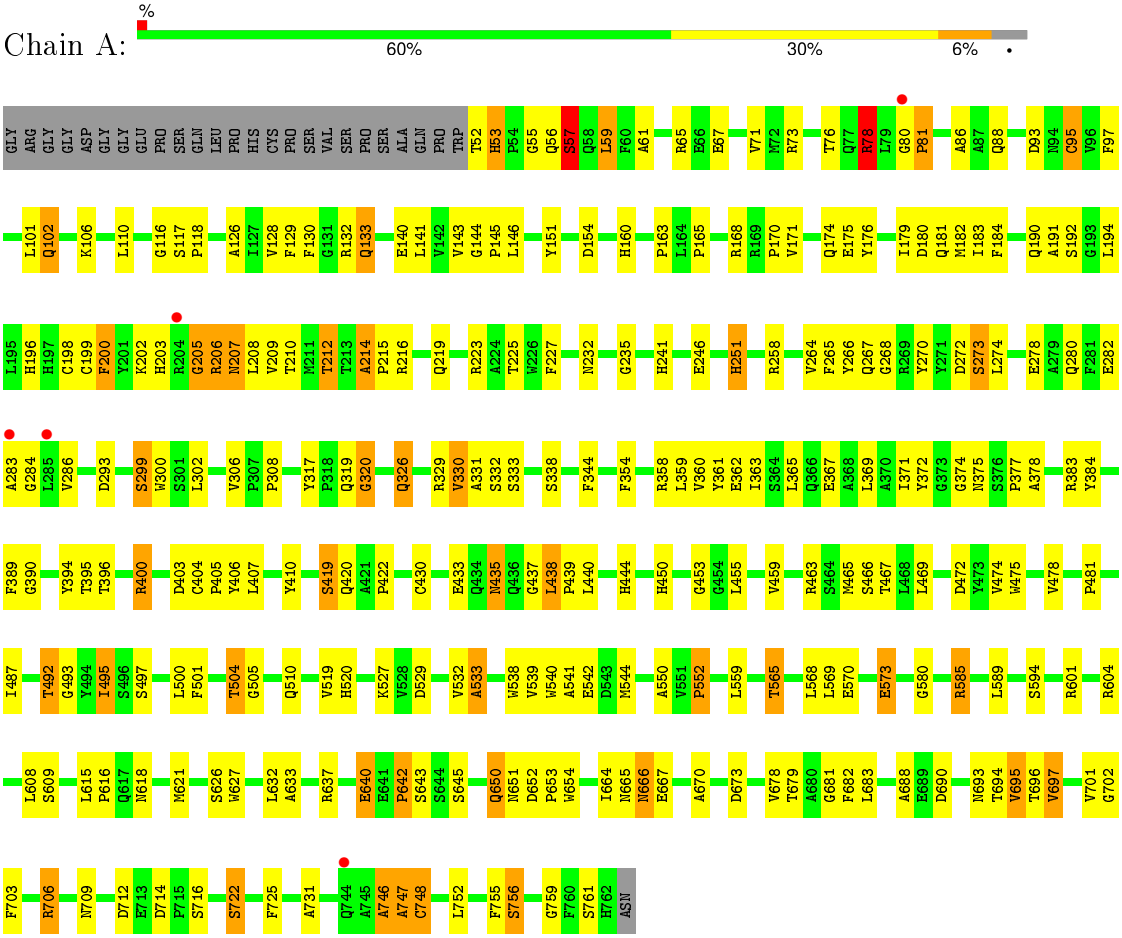
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	64	Total O 64 64	0	0
9	B	42	Total O 42 42	0	0

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.

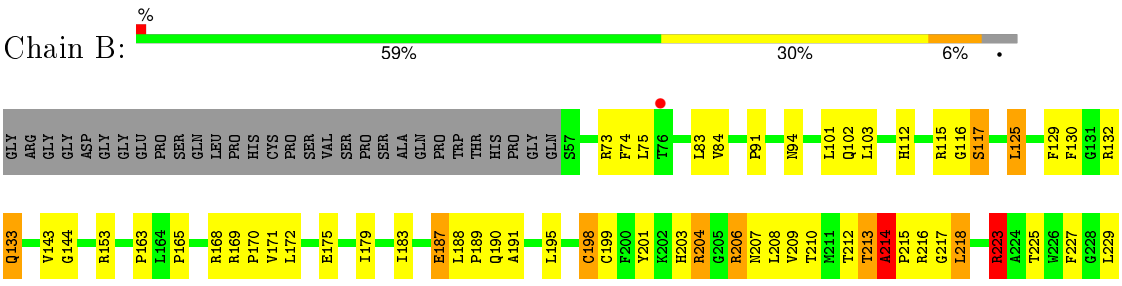
- Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

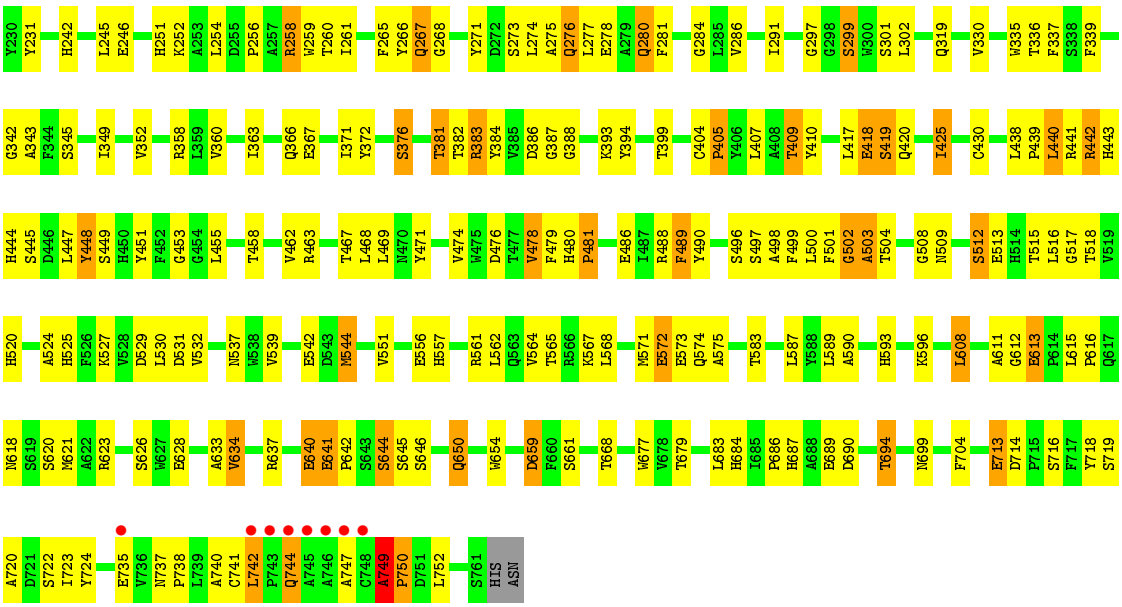
Chain A:



- Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

Chain B:




Y230 Y231 H242 L245 E246 H251 K252 A253 L254 D255 P256 A257 R258 W259 T260 I261 F265 Y266 Q267 G268 Y271 D272 S273 L274 A275 Q276 L277 E278 A279 Q280 F281 G284 L285 V286 I291 G297 G298 S299 W300 S301 L302 Q319 V330 W335 T336 F337 S338 F339
G342 A343 F344 S345 I349 V352 R358 L359 V360 I363 Q366 E367 I371 Y372 S376 T381 T382 R383 Y384 V385 D386 G387 G388 K393 Y394 T399 C404 P405 Y406 L407 A408 T409 Y410 L417 E418 S419 Q420 I425 C430 L438 P439 L440 R441 R442 H443
H444 S445 D446 L447 Y448 S449 H450 Y451 F452 G453 G454 L455 T458 V462 R463 T467 L468 L469 N470 Y471 V474 W475 D476 T477 V478 F479 H480 P481 E486 I487 R488 F489 Y490 S496 S497 A498 F499 L500 F501 G502 A503 T504 G508 N509 S512 E513 H514 T515 L516 G517 T518 V519
H520 A524 H525 F526 K527 V528 D529 L530 D531 V532 N537 W538 V539 E542 D543 M544 V551 E556 H557 R561 L562 Q563 V564 T565 R566 K567 L568 M571 E572 E573 Q574 A575 T583 L587 Y588 L589 A590 H593 K596 I608 A611 G612 E613 P614 L615 P616 Q617
N618 S619 S620 M621 A622 R623 S626 W627 E628 A633 V634 R637 E640 E641 P642 S643 S644 S645 S646 Q650 W654 D659 F660 S661 T668 W677 V678 T679 L683 H684 I685 P686 H687 A688 E689 D690 T694 N699 F704 E713 D714 P715 S716 F717 Y718 S719
A720 D721 S722 I723 Y724 E735 V736 N737 P738 L739 A740 C741 L742 P743 Q744 A745 A746 A747 C748 A749 P750 D751 L752 S761 HIS ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	226.47Å 226.47Å 219.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.39 – 2.80 49.34 – 2.80	Depositor EDS
% Data completeness (in resolution range)	77.9 (49.39-2.80) 77.9 (49.34-2.80)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.260 0.199 , 0.251	Depositor DCC
R_{free} test set	3176 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	1 of 63505 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11573	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, CA, JW7, TPQ, CU, MAN

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	0.73	1/5774 (0.0%)	0.95	6/7874 (0.1%)
1	B	0.73	2/5724 (0.0%)	0.93	8/7805 (0.1%)
All	All	0.73	3/11498 (0.0%)	0.94	14/15679 (0.1%)

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	A	0	3
1	B	0	4
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	641	GLU	CG-CD	6.26	1.61	1.51
1	B	641	GLU	CD-OE2	5.39	1.31	1.25
1	A	540	TRP	CB-CG	-5.39	1.40	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	223	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	78	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	529	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	531	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	223	ARG	NE-CZ-NH2	-5.91	117.34	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	CYS	Peptide
1	A	205	GLY	Peptide
1	A	437	GLY	Peptide
1	B	213	THR	Peptide
1	B	214	ALA	Peptide

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	5609	0	5351	171	1
1	B	5562	0	5313	197	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	39	0	34	1	0
5	A	28	0	25	0	0
5	B	28	0	25	0	0
6	A	28	0	26	0	0
6	B	56	0	52	2	0
7	A	25	0	20	4	0
7	B	25	0	20	6	0
8	B	61	0	52	3	0
9	A	64	0	0	1	0
9	B	42	0	0	8	0
All	All	11573	0	10918	353	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 16.

The worst 5 of 353 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:A:367:GLU:OE2	1:A:645:SER:OG	1.75	1.04
1:A:492:THR:HG21	1:B:441:ARG:HA	1.42	1.01
1:A:80:GLY:O	1:A:81:PRO:O	1.90	0.90
1:B:620:SER:HG	1:B:654:TRP:HD1	1.11	0.90
1:A:495:ILE:HB	9:A:2046:HOH:O	1.70	0.89

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)
1:A:326:GLN:OE1	1:A:326:GLN:OE1[10_665]	1.91	0.29

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	708/737 (96%)	599 (85%)	82 (12%)	27 (4%)	4 13
1	B	702/737 (95%)	607 (86%)	71 (10%)	24 (3%)	5 16
All	All	1410/1474 (96%)	1206 (86%)	153 (11%)	51 (4%)	4 14

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	116	GLY
1	A	206	ARG
1	A	214	ALA
1	A	267	GLN

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	590/610 (97%)	530 (90%)	60 (10%)	9 26
1	B	585/610 (96%)	519 (89%)	66 (11%)	7 22
All	All	1175/1220 (96%)	1049 (89%)	126 (11%)	8 24

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	722	SER
1	B	206	ARG
1	B	646	SER
1	A	756	SER
1	B	125	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	102	GLN
1	B	112	HIS
1	B	593	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPQ	A	471	1	13,14,15	1.49	2 (15%)	15,19,21	1.69	3 (20%)
1	TPQ	B	471	1	13,14,15	1.39	2 (15%)	15,19,21	1.59	2 (13%)

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
1	TPQ	A	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	471	1	-	0/4/22/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	TPQ	C6-C1	2.55	1.41	1.34
1	A	471	TPQ	C6-C1	2.66	1.41	1.34
1	B	471	TPQ	C3-C4	2.80	1.40	1.35
1	A	471	TPQ	C3-C4	3.57	1.41	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	TPQ	C3-C2-C1	-2.29	116.59	118.30
1	B	471	TPQ	O5-C5-C4	2.57	123.27	119.16
1	A	471	TPQ	C6-C1-C2	3.30	120.77	118.44
1	A	471	TPQ	O5-C5-C4	3.79	125.22	119.16
1	B	471	TPQ	C6-C1-C2	4.16	121.38	118.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	471	TPQ	1	0

5.5 Carbohydrates (i)

12 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	$\#\|Z\| > 2$
4	NAG	A	1765	1,4	14,14,15	0.71	0	15,19,21	1.61	3 (20%)
4	NAG	A	1766	4	14,14,15	0.80	1 (7%)	15,19,21	1.55	3 (20%)
4	BMA	A	1767	4	11,11,12	0.60	0	14,15,17	1.47	3 (21%)
5	NAG	A	1768	1,5	14,14,15	0.59	0	15,19,21	1.84	3 (20%)
5	NAG	A	1769	5	14,14,15	0.77	1 (7%)	15,19,21	1.43	3 (20%)
8	NAG	B	1765	1,8	14,14,15	0.55	0	15,19,21	1.13	0
8	NAG	B	1766	8	14,14,15	0.47	0	15,19,21	1.97	4 (26%)
8	BMA	B	1767	8	11,11,12	0.77	0	14,15,17	2.17	3 (21%)
8	BMA	B	1768	8	11,11,12	0.67	0	14,15,17	2.41	6 (42%)
8	MAN	B	1769	8	11,11,12	0.52	0	14,15,17	2.68	3 (21%)
5	NAG	B	1770	1,5	14,14,15	0.81	0	15,19,21	2.24	4 (26%)
5	NAG	B	1771	5	14,14,15	0.63	0	15,19,21	1.39	2 (13%)

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
4	NAG	A	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1767	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1768	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1769	5	-	0/6/23/26	0/1/1/1
8	NAG	B	1765	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1766	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1767	8	-	0/2/19/22	0/1/1/1
8	BMA	B	1768	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1769	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1770	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1771	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1766	NAG	O5-C1	-2.03	1.40	1.43
5	A	1769	NAG	C1-C2	2.04	1.55	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1767	BMA	O4-C4-C3	-4.83	99.46	110.34
8	B	1766	NAG	C2-N2-C7	-4.66	117.06	123.04
4	A	1766	NAG	O4-C4-C3	-3.60	102.22	110.34
4	A	1765	NAG	O4-C4-C3	-2.97	103.66	110.34
5	A	1768	NAG	C4-C3-C2	-2.83	106.83	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1765	NAG	1	0
8	B	1765	NAG	1	0
8	B	1767	BMA	2	0
8	B	1768	BMA	2	0

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	A	1770	1	14,14,15	1.16	2 (14%)	15,19,21	2.22	4 (26%)
6	NAG	A	1771	1	14,14,15	1.79	3 (21%)	15,19,21	3.00	7 (46%)
7	JW7	A	2000	-	23,28,28	1.86	3 (13%)	21,38,38	2.81	5 (23%)
6	NAG	B	1772	-	14,14,15	0.75	0	15,19,21	1.45	1 (6%)
6	NAG	B	1773	1	14,14,15	1.01	1 (7%)	15,19,21	2.75	3 (20%)
6	NAG	B	1774	1	14,14,15	1.49	1 (7%)	15,19,21	2.69	5 (33%)
6	NAG	B	1775	1	14,14,15	0.70	0	15,19,21	1.51	3 (20%)
7	JW7	B	2000	-	23,28,28	2.06	4 (17%)	21,38,38	2.82	7 (33%)

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	A	1770	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	1771	1	1/1/5/7	0/6/23/26	0/1/1/1
7	JW7	A	2000	-	-	0/9/20/20	0/4/4/4
6	NAG	B	1772	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1773	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1774	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	1775	1	-	0/6/23/26	0/1/1/1
7	JW7	B	2000	-	-	0/9/20/20	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2000	JW7	CAV-CAU	-5.56	1.39	1.49
7	B	2000	JW7	CAS-NAY	-5.22	1.33	1.44
7	A	2000	JW7	CAV-CAU	-5.01	1.40	1.49
7	A	2000	JW7	CAS-NAY	-4.45	1.34	1.44
7	B	2000	JW7	NAR-NAO	2.02	1.42	1.37

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2000	JW7	NAN-CAU-NAO	-11.12	105.96	114.88
7	B	2000	JW7	NAN-CAU-NAO	-9.21	107.49	114.88
6	B	1773	NAG	O7-C7-C8	-3.84	115.02	122.06
6	A	1771	NAG	O7-C7-C8	-3.84	115.02	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	2000	JW7	CAM-CAX-CAL	-3.64	104.62	110.82

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1770	NAG	C1
6	B	1774	NAG	C1
6	A	1771	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2000	JW7	4	0
6	B	1773	NAG	1	0
6	B	1774	NAG	1	0
7	B	2000	JW7	6	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, 95^{th} 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	710/737 (96%)	-0.49	5 (0%)	89	84	39, 58, 82, 138	0
1	B	704/737 (95%)	-0.41	9 (1%)	79	71	38, 59, 91, 153	0
All	All	1414/1474 (95%)	-0.45	14 (0%)	84	77	38, 59, 86, 153	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	746	ALA	5.3
1	B	747	ALA	5.0
1	B	745	ALA	4.2
1	B	748	CYS	3.0
1	B	735	GLU	2.9

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

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, 95^{th} 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
1	TPQ	B	471	14/15	0.98	0.26	-	44,53,56,59	0
1	TPQ	A	471	14/15	0.98	0.19	-	43,48,52,54	0

6.3 Carbohydrates

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, 95^{th} 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
5	NAG	A	1769	14/15	0.88	0.18	0.52	91,112,124,126	0
4	NAG	A	1765	14/15	0.97	0.13	-0.28	65,71,75,77	0
5	NAG	B	1770	14/15	0.95	0.11	-0.74	70,86,93,104	0
5	NAG	A	1768	14/15	0.98	0.10	-0.96	72,83,99,101	0
8	NAG	B	1765	14/15	0.98	0.09	-1.62	49,56,59,66	0
8	MAN	B	1769	11/12	0.89	0.31	-	112,126,141,142	0
5	NAG	B	1771	14/15	0.91	0.17	-	105,119,128,130	0
4	NAG	A	1766	14/15	0.94	0.18	-	63,76,95,112	0
8	BMA	B	1767	11/12	0.89	0.19	-	116,126,135,160	0
4	BMA	A	1767	11/12	0.76	0.30	-	110,116,124,128	0
8	BMA	B	1768	11/12	0.72	0.26	-	116,140,161,163	0
8	NAG	B	1766	14/15	0.91	0.18	-	67,101,115,119	0

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, 95^{th} 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
7	JW7	A	2000	25/25	0.91	0.29	4.58	65,90,143,148	0
7	JW7	B	2000	25/25	0.96	0.19	1.00	46,54,97,99	0
3	CA	A	1763	1/1	0.96	0.06	-1.26	51,51,51,51	0
3	CA	B	1763	1/1	0.98	0.06	-1.41	51,51,51,51	0
3	CA	B	1764	1/1	0.98	0.03	-3.40	60,60,60,60	0
3	CA	A	1764	1/1	0.93	0.04	-4.32	59,59,59,59	0
2	CU	A	1762	1/1	1.00	0.20	-	54,54,54,54	0
6	NAG	B	1775	14/15	0.84	0.28	-	72,97,107,109	0
6	NAG	A	1770	14/15	0.84	0.31	-	74,93,115,115	0
6	NAG	B	1773	14/15	0.79	0.23	-	87,129,136,136	0
2	CU	B	1762	1/1	1.00	0.18	-	54,54,54,54	0
6	NAG	A	1771	14/15	0.82	0.24	-	77,97,104,105	0
6	NAG	B	1772	14/15	0.73	0.31	-	103,132,140,141	0
6	NAG	B	1774	14/15	0.55	0.40	-	94,121,135,136	0

6.5 Other polymers (i)

There are no such residues in this entry.